Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.16 Developers Manual

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Abstract

The Dakota toolkit provides a flexible and extensible interface between simulation codes and iterative analysis methods. Dakota contains algorithms for optimization with gradient and nongradient-based methods; uncertainty quantification with sampling, reliability, and stochastic expansion methods; parameter estimation with nonlinear least squares methods; and sensitivity/variance analysis with design of experiments and parameter study methods. These capabilities may be used on their own or as components within advanced strategies such as surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty. By employing object-oriented design to implement abstractions of the key components required for iterative systems analyses, the Dakota toolkit provides a flexible and extensible problem-solving environment for design and performance analysis of computational models on high performance computers.

This report describes the Dakota class hierarchies. It is derived from annotation of the source code and provides detailed class documentation, including all member functions and attributes.

Contents

Chapter 1

Dakota Developers Manual

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1.1 Introduction

The Dakota software (`http://dakota.sandia.gov/`) delivers advanced parametric analysis techniques enabling quantification of margins and uncertainty, risk analysis, model calibration, and design exploration with computational models. Dakota contains algorithms for optimization with gradient and nongradient-based methods, uncertainty quantification with sampling, reliability, stochastic expansion, and interval estimation methods, parameter estimation with nonlinear least squares methods, and sensitivity/variance analysis with design of experiments and parameter study capabilities. (Solution verification and Bayesian approaches are also in development.) These capabilities may be used on their own or as components within advanced algorithms such as surrogate-based optimization, mixed integer nonlinear programming, mixed aleatory-epistemic uncertainty quantification, or optimization under uncertainty. By employing object-oriented design to implement abstractions of the key components required for iterative systems analyses, the Dakota toolkit provides a flexible problem-solving environment for design and performance analysis of computational models on high performance computers.

The Developers Manual focuses on documentation of Dakota design principles and class structures; it derives principally from annotated source code. For information on input command syntax, refer to the Reference Manual [1], and for more details on Dakota features and capabilities, refer to the Users Manual.

1.2 Overview of Dakota

In Dakota, the *environment* manages execution modes and input/output streams and defines the top-level iterator. This top-level iterator may be either a standard iterator or a meta-iterator. In the former case, the iterator identifies a model and the environment executes the iterator on the model to perform a single study. In the latter case, iterator recursions are present and sub-iterators may identify their own models. In both cases, models may contain additional recursions in the case of nested iteration or surrogate modeling. In a simple example, a hybrid meta-iterator might manage a global optimizer operating on a low-fidelity model that feeds promising design points into a local optimizer operating on a high-fidelity model. And in a more advanced example, a surrogate-based optimization under uncertainty approach would employ an uncertainty quantification iterator nested within an optimization iterator and would employ truth models contained within surrogate models. Thus, iterators and models provide both stand-alone capabilities as well as building blocks for more sophisticated studies.

A model contains a set of *variables*, an *interface*, and a set of *responses*, and the iterator operates on the model to map the variables into responses using the interface. Each of these components is a flexible abstraction with a variety of specializations for supporting different types of iterative studies. In a Dakota input file, the user specifies these components through environment, method, model, variables, interface, and responses keyword specifications.

The use of class hierarchies provides a mechanism for extensibility in Dakota components. In each of the various class hierarchies, adding a new capability typically involves deriving a new class and providing a set of virtual function redefinitions. These redefinitions define the coding portions specific to the new derived class, with the common portions already defined at the base class. Thus, with a small amount of new code, the existing facilities can be extended, reused, and leveraged for new purposes. The following sections tour Dakota's class organization.

1.2.1 Environment

Class hierarchy: Environment.

Environments provide the top level abstraction for managing different execution modes and managing input and output streams. Specific environments include:

- ExecutableEnvironment: the environment for execution of Dakota as a stand-alone application.
- LibraryEnvironment: the environment for execution of Dakota as an embedded library service.

1.2.2 Iterators

Class hierarchy: Iterator. Iterator implementations may choose to split operations up into run-time phases as described in Understanding Iterator Flow.

The iterator hierarchy contains a variety of iterative algorithms for optimization, uncertainty quantification, nonlinear least squares, design of experiments, and parameter studies. The hierarchy is divided into MetaIterator, Minimizer, and Analyzer branches.

The MetaIterator classes manage sequencing and collaboration among multiple methods with support for concurrent iterator parallelism. Methods include:

- SeqHybridMetaIterator: hybrid minimization using a set of iterators employing a corresponding set of models of varying fidelity. The sequential hybrid passes the best solutions from one method in as the starting points of the next method in the sequence.
- CollabHybridMetaIterator: hybrid minimization employing collaboration and sharing of response data among methods during the course if iteration. This class is currently a placeholder.
- EmbedHybridMetaIterator: hybrid minimization involving periodic use of a local search method for refinement during the iteration of an outer global method. This class is currently a placeholder.
- ConcurrentMetaIterator: two similar algorithms are available: (1) multi-start iteration from several different starting points, and (2) pareto set optimization for several different multi-objective weightings. Employs a single iterator with a single model, but runs multiple instances of the iterator concurrently for different settings within the model.

The Minimizer classes address optimization and deterministic calibration and are grouped into:

- Optimization: Optimizer provides a base class for gradient-based (e.g., CONMINOptimizer and SNLLOptimizer) and derivative-free (e.g., NCSUOptimizer, JEGAOptimizer) optimization solvers. Most of these are wrappers for third-party libraries that implement the optimization algorithms. Classes APPSEvalMgr and COLINApplication provide the function evaluation interface for APPSOptimizer and COLINOptimizer, respectively.
- Parameter estimation: LeastSq provides a base class for NL2SOLLeastSq, a least-squares solver based on NL2SOL, SNLLLeastSq, a Gauss-Newton least-squares solver, and NLSSOLLeastSq, an SQP-based least-squares solver.

- Surrogate-based minimization (both optimization and nonlinear least squares): SurrBasedMinimizer provides a base class for SurrBasedLocalMinimizer, SurrBasedGlobalMinimizer, and EffGlobalMinimizer. The surrogate-based local and global methods employ a single iterator with any of the available SurrogateModel capabilities (local, multipoint, or global data fits or hierarchical approximations) and perform a sequence of approximate optimizations, each involving build, optimize, and verify steps. The efficient global method, on the other hand, hard-wires a recursion involving Gaussian process surrogate models coupled with the DIRECT global optimizer to maximize an expected improvement function.

The Analyzer classes are grouped into:

- Uncertainty quantification: NonD provides a base class for non-deterministic methods in several categories:
  - Sampling: NonDSampling is further specialized with the NonDLHSSampling class for Latin hypercube and Monte Carlo sampling, and a number of other classes supporting incremental and adaptive sampling such as NonDAdaptImpSampling for multi-modal adaptive importance sampling.
  - Reliability Analysis: NonDReliability is further specialized with local and global methods (NonDLocalReliability and NonDGlobalReliability). NonDPOFDarts implements a computational geometry-based reliability method.
  - Stochastic Expansions: NonDExpansion includes specializations for generalized polynomial chaos (NonDPolynomialChaos) and stochastic collocation (NonDStochCollocation) and is supported by the NonDIntegration helper class, which supplies cubature, tensor-product quadrature and Smolyak sparse grid methods (NonDCubature, NonDQuadrature, and NonDSparseGrid).
  - Bayesian Calibration: NonDCalibration provides a base class for nondeterministic calibration methods with specialization to Bayesian calibration in NonDBayesCalibration, and specific implementations such as NonDQUESOBayesCalibration.
  - NonDInterval provides a base class for epistemic interval-based UQ methods. Three interval analysis approaches are provided: LHS (NonDLHSInterval), efficient global optimization (NonDGlobalInterval), and local optimization (NonDLocalInterval). Each of these three has specializations for single interval and Dempster-Shafer Theory of Evidence approaches.
- Parameter studies and design of experiments: PStudyDACE provides a base class for ParamStudy, which provides capabilities for directed parameter space interrogation, PSUADEDesignCompExp, which provides access to the Morris One-At-a-Time (MOAT) method for parameter screening, and DDACEDesignCompExp and FSUDesignCompExp, which provide for parameter space exploration through design and analysis of computer experiments. NonDLHSSampling from the uncertainty quantification branch also supports design of experiments when in `active all` variables mode.
- Solution verification studies: Verification provides a base class for RichExtrapVerification (verification via Richardson extrapolation) and other solution verification methods in development.

1.2.3 Models

Class hierarchy: Model.

The model classes are responsible for mapping variables into responses when an iterator makes a function evaluation request. There are several types of models, some supporting sub-iterators and sub-models for enabling layered and nested relationships. When sub-models are used, they may be of arbitrary type so that a variety of recursions are supported.

- SimulationModel: variables are mapped into responses using a simulation-based Interface object. No sub-iterators or sub-models are used.
- SurrogateModel: variables are mapped into responses using an approximation. The approximation is built and/or corrected using data from a sub-model (the truth model) and the data may be obtained using a sub-iterator (a design of experiments iterator). SurrogateModel has two derived classes: DataFitSurrModel for data fit surrogates and HierarchSurrModel for hierarchical models of varying fidelity. The relationship of the sub-iterators and sub-models is considered to be "layered" since they are not used as part of every response evaluation on the top level model, but rather used periodically in surrogate update and verification steps.

- NestedModel: variables are mapped into responses using a combination of an optional Interface and a sub-iterator/sub-model pair. The relationship of the sub-iterators and sub-models is considered to be "nested" since they are used to perform a complete iterative study as part of every response evaluation on the top level model.
- RecastModel: recasts the inputs and outputs of a sub-model for the purposes of variable transformations (e.g., variable scaling, transformations to standardized random variables) and problem reformulation (e.g., multi-objective optimization, response scaling, augmented Lagrangian merit functions, expected improvement).

1.2.4 Variables

Class hierarchy: Variables.

The Variables class hierarchy manages design, aleatory uncertain, epistemic uncertain, and state *variable types* for continuous, discrete integer, and discrete real *domain types*. This hierarchy is specialized according to how the domain types are managed:

- MixedVariables: domain type distinctions are retained, such that separate continuous, discrete integer, and discrete real domain types are managed. This is the default Variable perspective, and draws its name from "mixed continuous-discrete" optimization.
- RelaxedVariables: domain types are combined through relaxation of discrete constraints; i.e., continuous and discrete variables are merged into continuous arrays through relaxation of integrality (for discrete integer ranges) or set membership (for discrete integer or discrete real sets) requirements. The branch and bound minimizer is the only method using this approach at present.

Whereas domain types are defined based on the derived Variables class selection, the selection of active variable types is handled within each of these derived classes using variable views. These permit different algorithms to work on different subsets of variables. Data shared among Variables instances is stored in SharedVariablesData. For details on managing variables, see Working with Variable Containers and Views.

The Constraints hierarchy manages bound, linear, and nonlinear constraints and utilizes the same specializations for managing bounds on the variables (see MixedVarConstraints and RelaxedVarConstraints).

1.2.5 Interfaces

Class hierarchy: Interface.

Interfaces provide access to simulation codes or, conversely, approximations based on simulation code data. In the simulation case, an ApplicationInterface is used. ApplicationInterface is specialized according to the simulation invocation mechanism, for which the following nonintrusive approaches are supported:

- SysCallApplicInterface: the simulation is invoked using a system call (the C function `system()`). Asynchronous invocation utilizes a background system call. Utilizes the CommandShell utility.
- ForkApplicInterface: the simulation is invoked using a fork (the `fork/exec/wait` family of functions). Asynchronous invocation utilizes a nonblocking fork.
- SpawnApplicInterface: for Windows, fork is replaced by spawn. Asynchronous invocation utilizes a nonblocking spawn.

Fork and Spawn are inherited from ProcessHandleApplicInterface and System and ProcessHandle are inherited from ProcessApplicInterface. A semi-intrusive approach is also supported by:

- DirectApplicInterface: the simulation is linked into the Dakota executable and is invoked using a procedure call. Asynchronous invocations will utilize nonblocking threads (capability not yet available). Specializations of the direct interface are implemented in MatlabInterface, PythonInterface, ScilabInterface, and (for built-in testers) TestDriverInterface, while examples of plugin interfaces for library mode in serial and parallel, respectively, are included in SerialDirectApplicInterface and ParallelDirectApplicInterface

Scheduling of jobs for asynchronous local, message passing, and hybrid parallelism approaches is performed in the ApplicationInterface class, with job initiation and job capture specifics implemented in the derived classes.

In the approximation case, global, multipoint, or local data fit approximations to simulation code response data can be built and used as surrogates for the actual, expensive simulation. The interface class providing this capability is

- ApproximationInterface: builds an approximation using data from a truth model and then employs the approximation for mapping variables to responses. This class contains an array of Approximation objects, one per response function, which support a variety of approximation types using the different Approximation derived classes. These include SurfpackApproximation (provides kriging, MARS, moving least squares, neural network, polynomial regression, and radial basis functions), GaussProcApproximation (Gaussian process models), PecosApproximation (multivariate orthogonal and Lagrange interpolation polynomials from Pecos), TANA3Approximation (two-point adaptive nonlinearity approximation), and TaylorApproximation (local Taylor series).

which is an essential component within the DataFitSurrModel capability described above in Models.

1.2.6 Responses

Class: Response.

The Response class provides an abstract data representation of response functions and their first and second derivatives (gradient vectors and Hessian matrices). These response functions can be interpreted as objective functions and constraints (optimization data set), residual functions and constraints (least squares data set), or generic response functions (uncertainty quantification data set). This class is not currently part of a class hierarchy, since the abstraction has been sufficiently general and has not required specialization.

1.3 Services

A variety of services and utilities are used in Dakota for parallel computing, failure capturing, restart, graphics, etc. An overview of the classes and member functions involved in performing these services is included here.

- Multilevel parallel computing: Dakota supports multiple levels of nested parallelism. A meta-iterator can manage concurrent iterators, each of which manages concurrent function evaluations, each of which manages concurrent analyses executing on multiple processors. Partitioning of these levels with MPI communicators is managed in ParallelLibrary and scheduling routines for the levels are part of IteratorScheduler, ApplicationInterface, and ForkApplicInterface.

- Option management: Global options controlling behavior are managed in ProgramOptions, with the help of command-line option parsing in CommandLineHandler.

- Parsing: Dakota employs NIDR (New Input Deck Reader) via Dakota::ProblemDescDB::parse_inputs to parse user input files. NIDR uses the keyword handlers in the NIDRProblemDescDB derived class to populate data within the ProblemDescDB base class, which maintains a DataEnvironment specification and lists of DataMethod, DataModel, DataVariables, DataInterface, and DataResponses specifications. Procedures for modifying the parsing subsystem are described in Instructions for Modifying Dakota's Input Specification.

- Failure capturing: Simulation failures can be trapped and managed using exception handling in ApplicationInterface and its derived classes.

- Restart: Dakota maintains a record of all function evaluations both in memory (for capturing any duplication) and on the file system (for restarting runs). Restart options are managed through ProgramOptions (with the help of CommandLineHandler); file management in OutputManager; and restart file insertions occur in ApplicationInterface. The `dakota_restart_util` executable, built from restart_util.cpp, provides a variety of services for interrogating, converting, repairing, concatenating, and post-processing restart files.

- Memory management: Dakota employs the techniques of reference counting and representation sharing through the use of letter-envelope and handle-body idioms (Coplien, "Advanced C++"). The former idiom provides for memory efficiency and enhanced polymorphism in the following class hierarchies: Environment, Iterator, Model, Variables, Constraints, Interface, ProblemDescDB, and Approximation. The latter idiom provides for memory efficiency in data-intensive classes which do not involve a class hierarchy. The Response and parser data (DataEnvironment, DataMethod, DataModel, DataVariables, DataInterface, and DataResponses) classes use this idiom. When managing reference-counted data containers (e.g., Variables or Response objects), it is important to properly manage shallow and deep copies, to allow for both efficiency and data independence as needed in a particular context.
- Graphics and Output: Dakota provides 2D iteration history graphics using Motif widgets. Graphics data can also be cataloged in a tabular data file for post-processing with 3rd party tools such as Matlab, Tecplot, etc. These capabilities are encapsulated within the Graphics class. An experimental results database is implemented in ResultsManager and ResultsDBAny. Options for controlling output and facilities for managing it are in OutputManager.

1.4 Development Practices and Guidance

The following links provide guidance for core software components or specific development activities:

- Coding Style Guidelines and Conventions - coding practices used by the Dakota development team.
- Instructions for Modifying Dakota's Input Specification - how to interact with NIDR and the associated Dakota classes.
- Interfacing with Dakota as a Library - embed Dakota as a service within your application.
- Understanding Iterator Flow - explanation of the full granularity of steps in Iterator execution.
- Performing Function Evaluations - an overview of the classes and member functions involved in performing function evaluations synchronously or asynchronously.
- Working with Variable Containers and Views - discussion of data storage for variables and explanation of active and inactive views of this data.
- Demo TPL - a README for bringing a new Third-Party Library (TPL) into Dakota

1.5 Additional Resources

Additional development resources include:

- The Dakota Developer Portal linked from `http://dakota.sandia.gov/content/developer-portal/` includes information on getting started as a developer and links to project management resources.
- Project web pages are maintained at `http://dakota.sandia.gov/` including links to frequently asked questions, documentation, publications, mailing lists, and other resources.
- A Quickstart for bringing a new Third-Party Library (TPL) into Dakota can be found in the Dakota source tree under $DAKOTA_SRC/packages/external/demo_tpl/README.md .

Chapter 2

Coding Style Guidelines and Conventions

2.1 Introduction

Common code development practices can be extremely useful in multiple developer environments. Particular styles for code components lead to improved readability of the code and can provide important visual cues to other developers. Much of this recommended practices document is borrowed from the CUBIT mesh generation project, which in turn borrows its recommended practices from other projects, yielding some consistency across Sandia projects. While not strict requirements, these guidelines suggest a best-practices starting point for coding in Dakota.

2.2 C++/c Style Guidelines

Style guidelines involve the ability to discern at a glance the type and scope of a variable or function.

2.2.1 Class and variable styles

Class names should be composed of two or more descriptive words, with the first character of each word capitalized, e.g.:

```
class ClassName;
```

Class member variables should be composed of two or more descriptive words, with the first character of the second and succeeding words capitalized, e.g.:

```
double classMemberVariable;
```

Temporary (i.e. local) variables are lower case, with underscores separating words in a multiple word temporary variable, e.g.:

```
int temporary_variable;
```

Constants (i.e. parameters) and enumeration values are upper case, with underscores separating words, e.g.:

```
const double CONSTANT_VALUE;
```

2.2.2 Function styles

Function names are lower case, with underscores separating words, e.g.:

```
int function_name();
```

There is no need to distinguish between member and non-member functions by style, as this distinction is usually clear by context. This style convention allows member function names which set and return the value of a similarly-named private member variable, e.g.:

```
int memberVariable;
void member_variable(int a) { // set
  memberVariable = a;
}
int member_variable() const { // get
  return memberVariable;
}
```

In cases where the data to be set or returned is more than a few bytes, it is highly desirable to employ const references to avoid unnecessary copying, e.g.:

```
void continuous_variables(const RealVector& c_vars) { // set
  continuousVariables = c_vars;
}
const RealVector& continuous_variables() const {      // get
  return continuousVariables;
}
```

Note that it is not necessary to always accept the returned data as a const reference. If it is desired to be able change this data, then accepting the result as a new variable will generate a copy, e.g.:

```
// reference to continuousVariables cannot be changed
const RealVector& c_vars = model.continuous_variables();
// local copy of continuousVariables can be changed
RealVector c_vars = model.continuous_variables();
```

2.2.3 Miscellaneous

Appearance of typedefs to redefine or alias basic types is isolated to a few header files (`data_types.h`, `template_defs.h`), so that issues like program precision can be changed by changing a few lines of typedefs rather than many lines of code, e.g.:

```
typedef double Real;
```

`xemacs` is the preferred source code editor, as it has C++ modes for enhancing readability through color (turn on "Syntax highlighting"). Other helpful features include "Paren highlighting" for matching parentheses and the "New Frame" utility to have more than one window operating on the same set of files (note that this is still the same edit session, so all windows are synchronized with each other). Window width should be set to 80 internal columns, which can be accomplished by manual resizing, or preferably, using the following alias in your shell resource file (e.g., .cshrc):

```
alias xemacs "xemacs -g 81x63"
```

where an external width of 81 gives 80 columns internal to the window and the desired height of the window will vary depending on monitor size. This window width imposes a coding standard since you should avoid line wrapping by continuing anything over 80 columns onto the next line.

Indenting increments are 2 spaces per indent and comments are aligned with the code they describe, e.g.:

```
void abort_handler(int code)
{
  int initialized = 0;
  MPI_Initialized(&initialized);
  if (initialized) {
    // comment aligned to block it describes
    int size;
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    if (size>1)
      MPI_Abort(MPI_COMM_WORLD, code);
    else
      exit(code);
  }
  else
    exit(code);
}
```

Also, the continuation of a long command is indented 2 spaces, e.g.:

```
const String& iterator_scheduling
  = problem_db.get_string("strategy.iterator_scheduling");
```

and similar lines are aligned for readability, e.g.:

```
cout << "Numerical gradients using " << finiteDiffStepSize*100. << "%"
     << finiteDiffType << " differences\nto be calculated by the "
     << methodSource << " finite difference routine." << endl;
```

Lastly, #ifdef's are not indented (to make use of syntax highlighting in xemacs).

2.3 File Naming Conventions

In addition to the style outlined above, the following file naming conventions have been established for the Dakota project.

File names for C++ classes should, in general, use the same name as the class defined by the file. Exceptions include:

- with the introduction of the Dakota namespace, base classes which previously utilized prepended Dakota identifiers can now safely omit the identifiers. However, since file names do not have namespace protection from name collisions, they retain the prepended Dakota identifier. For example, a class previously named DakotaModel which resided in DakotaModel.cpp/hpp, is now Dakota::Model (class Model in namespace Dakota) residing in the same filenames. The retention of the previous filenames reduces the possibility of multiple instances of a Model.hpp causing problems. Derived classes (e.g., NestedModel) do not require a prepended Dakota identifier for either the class or file names.
- in a few cases, it is convenient to maintain several closely related classes in a single file, in which case the file name may reflect the top level class or some generalization of the set of classes (e.g., DakotaResponse.[CH] files contain Dakota::Response and Dakota::ResponseRep classes, and DakotaBinStream.[CH] files contain the Dakota::BiStream and Dakota::BoStream classes).

The type of file is determined by one of the four file name extensions listed below:

- **.hpp** A class header file ends in the suffix .hpp. The header file provides the class declaration. This file does not contain code for implementing the methods, except for the case of inline functions. Inline functions are to be placed at the bottom of the file with the keyword inline preceding the function name.
- **.cpp** A class implementation file ends in the suffix .cpp. An implementation file contains the definitions of the members of the class.
- **.h** A header file ends in the suffix .h. The header file contains information usually associated with procedures. Defined constants, data structures and function prototypes are typical elements of this file.
- **.c** A procedure file ends in the suffix .c. The procedure file contains the actual procedures.

2.4 Class Documentation Conventions

Class documentation uses the doxygen tool available from `http://www.doxygen.org` and employs the JAVA-doc comment style. Brief comments appear in header files next to the attribute or function declaration. Detailed descriptions for functions should appear alongside their implementations (i.e., in the .cpp files for non-inlined, or in the headers next to the function definition for inlined). Detailed comments for a class or a class attribute must go in the header file as this is the only option.

NOTE: Previous class documentation utilities (class2frame and class2html) used the "//-" comment style and comment blocks such as this:

```
//- Class:       Model
//- Description: The model to be iterated by the Iterator.
//-              Contains Variables, Interface, and Response objects.
//- Owner:       Mike Eldred
//- Version: $Id: Dev_Recomm_Pract.dox 4549 2007-09-20 18:25:03Z mseldre $
```

These tools are no longer used, so remaining comment blocks of this type are informational only and will not appear in the documentation generated by doxygen.

2.5 CMake Style Guidelines

Dakota conventions for CMake files, such as CMakeLists.txt, FooConfig.cmake, etc., follow. Our goal is ease of reading, maintenance, and support, similar to the C++ code itself. Current CMake versions and build hints are maintained at the Developer Portal http://dakota.sandia.gov/developer/.

2.5.1 CMake Code Formatting

- Indentation is 2 spaces, consistent with Dakota C++ style.
- Lines should be kept to less than 80 chars per line where possible.
- Wrapped lines may be indented two spaces or aligned with prior lines.
- For ease of viewing and correctness checking in Emacs, a customization file is available: http://www.cmake.org/CMakeDocs/cmake-mode.el

2.5.2 CMake Variable Naming Conventions

These variable naming conventions are especially important for those that ultimately become preprocessor defines and affect compilation of source files.

- Classic/core elements of the CMake language are set in lower_case, e.g., option, set, if, find_library.
- Static arguments to CMake functions and macros are set in UPPER_CASE, e.g. REQUIRED, NO_MODULE, QUIET.
- Minimize "global" variables, i.e., don't use 2 variables with the same meaning when one will do the job.
- Feature toggling: when possible, use the "HAVE_<pkg/feature>" convention already in use by many CMake-enabled TPLs, e.g.,

```
$ grep HAVE_SYSTEM Dakota/src/CMakeLists.txt

check_function_exists(system HAVE_SYSTEM)
if(HAVE_SYSTEM)
  add_definitions("-DHAVE_SYSTEM")
endif(HAVE_SYSTEM)

$ grep HAVE_CONMIN Dakota/src/CMakeLists.txt Dakota/packages/CMakeLists.txt
Dakota/src/CMakeLists.txt:if(HAVE_CONMIN)
Dakota/src/CMakeLists.txt:endif(HAVE_CONMIN)
Dakota/packages/CMakeLists.txt:option(HAVE_CONMIN "Build the CONMIN package." ON)
Dakota/packages/CMakeLists.txt:if(HAVE_CONMIN)
Dakota/packages/CMakeLists.txt:endif(HAVE_CONMIN)
```

- When a variable/preprocessor macro could result in name clashes beyond Dakota scope, e.g., for library_mode users, consider prefixing the "HAVE_<pkg>" name with DAKOTA_, e.g. DAKOTA_HAVE_MPI. Currently, MPI is the only use case for such a variable in Dakota, but many examples can be found in the CMake Modules source, e.g.

```
grep _HAVE_ <cmake_prefix_dir>/share/cmake-2.8/Modules/*
```

Chapter 3

Instructions for Modifying Dakota's Input Specification

To modify Dakota's input specification (for maintenance or addition of new input syntax), specification maintenance mode must be enabled at Dakota configure time with the `-DENABLE_SPEC_MAINT` option, e.g.,

```
./cmake -DENABLE_SPEC_MAINT:BOOL=ON ..
```

This will enable regeneration of NIDR and Dakota components which must be updated following a spec change.

3.1 XML Input Specification

The authoritative source for valid Dakota input grammar is `dakota/src/dakota.xml`. The schema defining valid content for this XML file is in `dakota/src/dakota.xsd`. NIDR remains Dakota's user input file parser, so `dakota.xml` is translated to `dakota/src/dakota.input.nspec` during the Dakota build process. To update the XML input definition:

- Make sure ENABLE_SPEC_MAINT is enabled in your build and necessary Java development tools are installed (see below).
- Edit the XML spec in `dakota.xml`.
- Perform a make in `dakota.build/src` which will regenerate `dakota.source/src/dakota`.input.-nspec and related file.
- Review that any changes induced in the `dakota.input.nspec` file are as expected.
- Proceed with verifying code changes and making downstream parse handler changes as normal (described below).
- Commit the modified `dakota.xml`, `dakota.input.nspec`, and other files generated to `dakota.-source/src` along with your other code changes.

3.1.1 XML Build Requirements

Editing the XML and then compiling Dakota requires

- Java Development Kit (JDK) providing the Java compiler javac. Java 6 (version 1.6) or newer should work, with Java 8 recommended. Can satisfy on RHEL6 with RPM packages `java-1.8.0-openjdk-devel` and `java-1.8.0-openjdk`. This is needed to build the Java-based XML to NIDR translator. If this becomes too burdensome, we can check in the generated `xml2nidr.jar` file.

3.1.2 XML Editing Tools

The following tools will make editing dakota.input.xml easier.

- **Recommended: Eclipse Web Tools Platform.** Includes both graphical and text editors.
  1. Download Eclipse Standard (Classic)
  2. Configure proxy if needed, setting to manual: Window > Preferences > General > Network Connection > Proxy
  3. Install Web Tools Platform
     - Help > Install New Software
     - Work With: Kepler - `http://download.eclipse.org/releases/kepler`
     - Search "Eclipse X" and install two packages under Web, XML, Java
       * Eclipse XML Editors and Tools
       * Eclipse XSL Developer Tools
     - Optionally install C/C++ Development Tools
  4. Optional: add Subclipse for subversion (Subversive is the other major competing tool and I don't think requires JavaHL) Help > Install New Software Work With: `http://subclipse.tigris.org/update_1.6.x` Install Subclipse On Linux: yum install subversion-javahl.x86_64
  5. Alternately install Eclipse for Java or Eclipse Java EE development which includes webtools, then optionally add subclipse and C/C++ dev
- **Alternate: Emacs or your usual editor.** For example, Emacs supports an Nxml mode. You can tell it where to find the schema, edit XML, and have it perform validation against the schema. See help at `http://www.gnu.org/software/emacs/manual/html_mono/nxml-mode.html`
- **Other Suggested Alternates:** XMLSpy, DreamWeaver, XML Copy Editor

3.1.3 XML Features (with map to NIDR)

Out of necessity, Dakota XML `dakota.xml` closely mirrors `dakota.input.nspec`. Valid Dakota input grammar is constrained by `dakota.xml`, an XML document which must validate against `dakota.xsd`. The top-level element of interest is <input>, which is comprised of a sequence of content elements (keywords, alternates, etc.), which may themselves contain additional child content elements. The key content types are:

- **Keyword (<keyword>):**, specified with the <keyword> element whose definition is given by keywordType in `dakota.xsd`. The required attributes are:
  - **name:** The keyword name (lower case with underscores) as it will be given in user input; must follow same uniqueness rules are historical NIDR. User input is allowed in mixed case, but the XML must use lower case names.

    Since the NIDR parser allows keyword abbreviation, you *must* not add a keyword that could be misinterpreted as an abbreviation for a different keyword within the same top-level keyword, such as "environment" and "method". For example, adding the keyword "expansion" within the method specification would be a mistake if the keyword "expansion_factor" already was being used in this block.

    The NIDR input is somewhat order-dependent, allowing the same keyword to be reused multiple times in the specification. This often happens with aliases, such as `lower_bounds`, `upper_bounds` and `initial_point`. Ambiguities are resolved by attaching a keyword to the most recently seen context in which it could appear, if such exists, or to the first relevant context that subsequently comes along in the input file.
  - **code:** The verbatim NIDR handler to be invoked when this keyword parsed. In NIDR this was specified with {N_macro(...)}.

  Optional/useful parser-related elements/attributes in order of importance are:

- **param sub-element:**Parameters and data types: A keyword may have an associated parameter element with a specified data type: `<param type="PARAMTYPE" />`. NIDR data types remain the same (INTEGER, REAL, STRING and LISTs thereof, but new data types INPUT_FILE and OUTPUT_FILE add convenience for the GUI, mapping to STRING for NIDR purposes. Parameters can also include attributes `constraint`, `in_taglist`, or `taglist`, which are used to help validate the user-specified parameter value. For example `constraint >= 0 LEN normal_uncertain`
- **alias sub-element:** Historical aliases for this keyword (can appear multiple times). Alias has a single attribute **name** which must be lower case with underscores.
- **id:** Unique ID for the keyword, usually name with an integer appended, but not currently used/enforced.
- **minOccurs:** Minimum occurrences of the keyword in current context (set to 1 for required, 0 for optional)
- **maxOccurs:** Maximum occurrences of the keyword in current context (for example environment may appear at most once)

And optional/useful GUI-related attributes are:

- **help:** (Don't add this attribute the new keywords!) A pointer to the corresponding reference manual section (deprecated as not needed with new reference manual format which mirrors keyword hierarchy).
- **label:** a short, friendly label string for the keyword in the GUI. Format these like titles, e.g., "Initial Point for Search".
- **group:** Category or group for this keyword, e.g., optimization vs. parameter study if they are to be groups for GUI purposes

• **Alternation (<oneOf>):** Alternation of groups of content is done with the element <oneOf> which indicates that its immediate children are alternates. In NIDR this was done with the pipe symbol: OptionA | OptionB. oneOf allows the label attribute and its use is recommended.

• **Required Group (<required>):** A required group can be specified by enclosing the contents in the <required> element. In NIDR this was done by enclosing the content in parentheses: (required group...)

• **Optional Group (<optional>):** An optional group can be specified by enclosing the contents in the <optional> element. In NIDR this was done by enclosing the content in brackets: [optional group...]

3.2 Rebuild Generated Files

When configured with `-DENABLE_SPEC_MAINT`, performing a make in `dakota.build/src` will regenerate all files which derive from `dakota.xml`, include dakota.input.nspec, NIDR_keywds.hpp, and dakota.input.summary. If you commit changes to a source repository, be sure to commit any automatically generated files in addition to any modified in the following steps. It is not strictly necessary to run make at this point in the sequence, and in fact may generate errors if necessary handlers aren't yet available.

Warning

Please do not manually modify generated files!

3.3 Update Parser Source NIDRProblemDescDB.cpp

Many keywords have data associated with them: an integer, a floating-point number, a string, or arrays of such entities. Data requirements are specified in dakota.input.nspec by the tokens INTEGER, REAL, STRING, INTEGERLIST, REALLIST, STRINGLIST. (Some keywords have no associated data and hence no such token.) After each keyword and data token, the dakota.input.nspec file specifies functions that the NIDR parser should call to record the appearance of the keyword and deal with any associated data. The general form of this specification is

{ startfcn, startdata, stopfcn, stopdata }

i.e., a brace-enclosed list of one to four functions and data pointers, with trailing entities taken to be zero if not present; zero for a function means no function will be called. The startfcn must deal with any associated data.

Otherwise, the distinction between startfcn and stopfcn is relevant only to keywords that begin a group of keywords (enclosed in parentheses or square brackets). The startfcn is called before other entities in the group are processed, and the stop function is called after they are processed. Top-level keywords often have both startfcn and stopfcn; stopfcn is uncommon but possible for lower-level keywords. The startdata and (if needed) stopdata values are usually pointers to little structures that provide keyword-specific details to generic functions for startfcn and stopfcn. Some keywords that begin groups (such as "approx_problem" within the top-level "environment" keyword) have no need of either a startfcn or a stopfcn; this is indicated by "{0}".

Most of the things within braces in dakota.input.nspec are invocations of macros defined in `dakota.-source/src/NIDRProblemDescDB`.cpp. The macros simplify writing dakota.input.nspec and make it more readable. Most macro invocations refer to little structures defined in NIDRProblemDescDB.cpp, usually with the help of other macros, some of which have different definitions in different parts of NIDRProblemDescDB.cpp. When adding a keyword to dakota.input.nspec, you may need to add a structure definition or even introduce a new data type. NIDRProblemDescDB.cpp has sections corresponding to each top-level keyword. The top-level keywords are in alphabetical order, and most entities in the section for a top-level keyword are also in alphabetical order. While not required, it is probably good practice to maintain this structure, as it makes things easier to find.

Any integer, real, or string data associated with a keyword are provided to the keyword's startfcn, whose second argument is a pointer to a `Values` structure, defined in header file `nidr.h`.

Example 1: if you added the specification:

```
[method_setting REAL {method_setting_start, &method_setting_details} ]
```

you would provide a function

```
    void NIDRProblemDescDB::
method_setting_start(const char *keyname, Values *val, void **g, void *v)
{ ... }
```

in NIDRProblemDescDB.cpp. In this example, argument `&method_setting_details` would be passed as `v`, `val->n` (the number of values) would be 1 and `*val->r` would be the REAL value given for the `method-_setting` keyword. The `method_setting_start` function would suitably store this value with the help of `method_setting_details`.

For some top-level keywords, `g` (the third argument to the startfcn and stopfcn) provides access to a relevant context. For example, `method_start` (the startfcn for the top-level `method` keyword) executes

```
DataMethod *dm = new DataMethod;
 g = (void*)dm;
```

(and supplies a couple of default values to `dm`). The start functions for lower-level keywords within the `method` keyword get access to `dm` through their `g` arguments. Here is an example:

```
 void NIDRProblemDescDB::
method_str(const char *keyname, Values *val, void **g, void *v)
{
        (*(DataMethod**)g)->**(String DataMethod::**)v = *val->s;
        }
```

In this example, `v` points to a pointer-to-member, and an assignment is made to one of the components of the DataMethod object pointed to by `*g`. The corresponding stopfcn for the top-level `method` keyword is

```
 void NIDRProblemDescDB::
method_stop(const char *keyname, Values *val, void **g, void *v)
{
        DataMethod *p = *(DataMethod**)g;
        pDDBInstance->dataMethodList.insert(*p);
        delete p;
        }
```

which copies the now populated DataMethod object to the right place and cleans up.

Example 2: if you added the specification

```
[method_setting REALLIST {{N_mdm(RealL,methodCoeffs)}
```

then method_RealL (defined in NIDRProblemDescDB.cpp) would be called as the startfcn, and methodCoeffs would be the name of a (currently nonexistent) component of DataMethod. The N_mdm macro is defined in NIDRProblemDescDB.cpp; among other things, it turns `RealL` into `NIDRProblemDescDB::method_RealL`. This function is used to process lists of REAL values for several keywords. By looking at the source, you can see that the list values are val->r[i] for 0 <= `i` < val->n.

3.4 Update Corresponding Data Classes

The Data classes (DataEnvironment, DataMethod, DataModel, DataVariables, DataInterface, and DataResponses) store the parsed user input data. In this step, we extend the Data class definitions to include any new attributes referred to in `dakota.xml` or `NIDRProblemDescDB`

3.4.1 Update the Data Class Header File

Add a new attribute to the public data for each of the new specifications. Follow the style guide for class attribute naming conventions (or mimic the existing code).

3.4.2 Update the .cpp File

Define defaults for the new attributes in the constructor initialization list (if not a container with a sensible default constructor) in same order as they appear in the header. Add the new attributes to the write(MPIPackBuffer&), read(-MPIUnpackBuffer&), and write(ostream&) functions, paying careful attention to the use of a consistent ordering.

3.5 Update Database Source ProblemDescDB.cpp

3.5.1 Augment/update get_<data_type>() Functions

The next update step involves extending the database retrieval functions in `dakota.source/src/ProblemDescDB`.cpp. These retrieval functions accept an identifier string and return a database attribute of a particular type, e.g., a RealVector:

```
const RealVector& get_rv(const String& entry_name);
```

The implementation of each of these functions contains tables of possible entry_name values and associated pointer-to-member values. There is one table for each relevant top-level keyword, with the top-level keyword omitted from the names in the table. Since binary search is used to look for names in these tables, each table must be kept in alphabetical order of its entry names. For example,

```
...
else if ((L = Begins(entry_name, "model."))) {
  if (dbRep->methodDBLocked)
      Locked_db();

  #define P &DataModelRep::
  static KW<RealVector, DataModelRep> RVdmo[] = {      // must be sorted
      {"nested.primary_response_mapping", P primaryRespCoeffs},
      {"nested.secondary_response_mapping", P secondaryRespCoeffs},
      {"surrogate.kriging_conmin_seed", P krigingConminSeed},
      {"surrogate.kriging_correlations", P krigingCorrelations},
      {"surrogate.kriging_max_correlations", P krigingMaxCorrelations},
      {"surrogate.kriging_min_correlations", P krigingMinCorrelations}};
  #undef P

  KW<RealVector, DataModelRep> *kw;
  if ((kw = (KW<RealVector, DataModelRep>*)Binsearch(RVdmo, L)))
      return dbRep->dataModelIter->dataModelRep->*kw->p;
}
```

is the "model" portion of ProblemDescDB::get_rv(). Based on entry_name, it returns the relevant attribute from a DataModel object. Since there may be multiple model specifications, the `dataModelIter` list iterator identifies which node in the list of DataModel objects is used. In particular, `dataModelList` contains a list of all of the `data_model` objects, one for each time a top-level `model` keyword was seen by the parser. The particular model object used for the data retrieval is managed by `dataModelIter`, which is set in a `set_db_list_nodes()` operation that will not be described here.

There may be multiple DataMethod, DataModel, DataVariables, DataInterface, and/or DataResponses objects. However, only one specification is currently allowed so a list of DataEnvironment objects is not needed. Rather, ProblemDescDB::environmentSpec is the lone DataEnvironment object.

To augment the get_<data_type>() functions, add table entries with new identifier strings and pointer-to-member values that address the appropriate data attributes from the Data class object. The style for the identifier strings is a top-down hierarchical description, with specification levels separated by periods and words separated with underscores, e.g., `"keyword.group_specification.individual_specification"`. Use the `dbRep->listIter->attribute` syntax for variables, interface, responses, and method specifications. For example, the `method_setting` example attribute would be added to `get_drv()` as:

```
{"method_name.method_setting", P methodSetting},
```

inserted at the beginning of the `RVdmo` array shown above (since the name in the existing first entry, i.e., "nested.-primary_response_mapping", comes alphabetically after "method_name.method_setting").

3.6 Use get_<data_type>() Functions

At this point, the new specifications have been mapped through all of the database classes. The only remaining step is to retrieve the new data within the constructors of the classes that need it. This is done by invoking the get-_<data_type>() function on the ProblemDescDB object using the identifier string you selected in Augment/update get_<data_type>() Functions. For example:

```
const String& interface_type = problem_db.get_string("interface.type");
```

passes the `"interface.type"` identifier string to the ProblemDescDB::get_string() retrieval function, which returns the desired attribute from the active DataInterface object.

Warning

> Use of the get_<data_type>() functions is restricted to class constructors, since only in class constructors are the data list iterators (i.e., `dataMethodIter`, `dataModelIter`, `dataVariablesIter`, `dataInterfaceIter`, and `dataResponsesIter`) guaranteed to be set correctly. Outside of the constructors, the database list nodes will correspond to the last set operation, and may not return data from the desired list node.

3.7 Update the Documentation

Doxygen comments should be added to the Data class headers for the new attributes, and the reference manual sections describing the portions of `dakota.xml` that have been modified should be updated by updating files in `dakota.source/docs/KeywordMetaData/`. d`dakota.xml`, together with these metadata files generates the reference manual and GUI context-aware help documentation.

Chapter 4

Understanding Iterator Flow

This page explains the various phases comprising Iterator::run_iterator(). Prior to Iterator construction, when command-line options are parsed, Boolean run mode flags corresponding to PRERUN, RUN, and POSTRUN are set in ParallelLibrary. If the user didn't specify any specific run modes, the default is for all three to be true (all phases will execute).

Iterator is constructed.

When called, `run_iterator()` sequences:

- `initialize_run()`: unconditionally called, virtual. Performs common initialization such as allocating workspaces, setting communicators and evaluation counts. When re-implementing this virtual, a derived class must call its nearest parent's initialize_run(), typically *before* performing its own implementation steps.
- *Not implemented: pre-run input*
- IF PRERUN, invoke `pre_run()`: virtual function; default no-op. Purpose: derived classes should implement `pre_run()` if they are able to generate all parameter sets (variables) at once, separate from `run()`. Derived implementations should call their nearest parent's pre_run(), typically *before* performing their own steps.
- IF PRERUN, invoke `pre_output()`: non-virtual function; if user requested, output variables to file.
- *Not implemented: run input*
- IF RUN, invoke virtual function `run()`. Purpose: at a minimum, evaluate parameter sets through computing responses; for iterators without pre/post capability, their entire implementation is in `run()` and this is a reasonable default for new Iterators.
- *Not implemented: run output*
- IF POSTRUN, invoke `post_input()`: virtual function, default only print helpful message on mode. Purpose: derived iterators supporting post-run input from file must implement to read file and populate variables/responses (and possibly best points) appropriately. Implementations must check if the user requested file input.
- IF POSTRUN, invoke `post_run()`: virtual function. Purpose: generate statistics / final results. Any analysis that can be done solely on tabular data read by `post_input()` can be done here. Derived re-implementations should call their nearest parent's post-run(), typically *after* performing their specific post-run activities.
- *Not implemented: post-run output*
- `finalize_run()`: unconditionally called, virtual. Purpose: free workspaces. Default base class behavior is no-op, however, derived implementations should call their nearest parent's finalize_run *after* performing their specialized portions.

Iterator is destructed.

Chapter 5

Interfacing with Dakota as a Library

5.1 Introduction

Tightly integrating or linking Dakota into another application can improve user experience by delivering a more unified, inter-operable software tool for optimization and UQ analyses, improving performance by eliminating file system-based interfaces, and reducing challenges with parallel computing inter-operation. This benefit has been realized within several Sandia and external simulation applications. This section describes how to link Dakota into another C++ application.

Dakota has two primary application programming interfaces (APIs). The LibraryEnvironment class facilitates use of Dakota as an algorithm service library within another application. In this case, the simulation application is providing a "front end" for Dakota. The second API, provided by the DirectApplicInterface class, provides an interface for Dakota to call the simulation code directly to perform function evaluations in core. This permits the simulation to be the "back end" for Dakota. The most complete library integration of Dakota would use both in combination, with the overall simulation framework providing both the front end and back end for Dakota, creating a sandwich, as loosely depicted here:

```
[------------
[ Application
[
[   ( -----
[   ( Dakota (LibraryEnvironment)
[   (
[   (   { Function evaluation callback to Application (via DirectApplicInterface)
[   (   {   |
[ <------/
[   (   {
[   (
[   ( -----
[
[------------
```

Attention

> Dakota may be integrated as a library in other software applications subject to the terms of the GNU Lesser General Public License (LGPL). Refer to `http://www.gnu.org/licenses/lgpl.html` or the LICENSE file included with Dakota.

When Dakota is compiled and installed, the relevant library API headers are installed to `CMAKE_INSTALL_PREFIX/include` and the runtime libraries primarily to `CMAKE_INSTALL_PREFIX/lib/` (on some platforms, to `CMAKE_INSTALL_PREFIX/bin/`. The core C/C++ code is in the library `dakota_src`, while Fortran code lives in the `dakota_src_fortran` library. Information on using the API in Dakota headers is included throughout this section, while considerations for configuring and linking against Dakota and its various required and optional third–party libraries are emphasized in the section Linking against the Dakota library.

Steps involved in integrating Dakota into another application typically include:

1. Writing C++ code for your application to instantiate, configure, and execute Dakota's LibraryEnvironment ("front end"); see Basic Dakota library instantiation and Configuring Dakota operation.
2. Writing C++ code for Dakota to call a function in your application to perform function evaluations ("back end"); see Creating a simulator plugin interface.
3. Compiling Dakota and linking into your application (Linking against the Dakota library).

Several source code examples demonstrate Dakota library interfaces. The classes SIM::SerialDirectApplicInterface and SIM::ParallelDirectApplicInterface demonstrate serial and parallel simulation function evaluation plug-ins. The file library_mode.cpp includes a main program that exercises Dakota libraries in serial and parallel modes with these mock simulator programs, with various ways of configuring Dakota problem definition and operation. Finally, library_split.cpp demonstrates running Dakota as a library modular on an MPI sub-communicator.

5.2 Basic Dakota library instantiation

The function run_dakota_parse() in library_mode.cpp demonstrates the basic use of Dakota library objects as one would in another main application that embeds Dakota. In this example, Dakota is configured based on a typical user-provided text-based Dakota input file (the same that would be provided at the command line with `dakota -i dakota_optimization.in`) and a function evaluator derived from a DirectApplicInterface is plugged into the Dakota library environment.

First, an object of type ProgramOptions which manages top-level Dakota settings is instantiated and configured to specify the name of the Dakota user input file. Additional options for output and error redirection, restart operation, and more may be set via ProgramOptions. See its class documentation for details.

```
string dakota_input_file = "dakota_optimization.in";
Dakota::ProgramOptions opts;
opts.input_file(dakota_input_file);
```

Next, a LibraryEnvironment is created, passing the desired settings from opts:

```
Dakota::LibraryEnvironment env(opts);
```

This standard constructor will parse the specified input and create Dakota objects. It assumes many default settings, including that the parent application initialized MPI if running in parallel mode. (In this case, Dakota will detect whether MPI was initialized and not call MPI_Init or MPI_Finalize.) For more advanced use cases described below, alternate constructors allow constructing based on MPI communicators, with delayed finalization, and with Dakota database update function callbacks. Then the application's function evaluator implementing Dakota's DirectApplicInterface is plugged in with a convenience function serial_interface_plugin() or parallel_interface_plugin(). Finally, the Dakota analysis is run by calling

```
env.execute();
```

The next two sections offer additional details on (1) alternative and supplementary ways to configure Dakota's operation (Configuring Dakota operation) and (2) how to specialize Dakota's DirectApplicInterface to provide a function evaluator plugin to Dakota (Creating a simulator plugin interface).

Remarks

After LibraryEnvironment construction, all MPI communicator partitioning has been performed and the ParallelLibrary instance may be interrogated for parallel configuration data. For example, the lowest level communicators in Dakota's multilevel parallel partitioning are the analysis communicators, which can be retrieved using:

```
// retrieve the set of analysis communicators for simulation initialization:
// one analysis comm per ParallelConfiguration (PC), one PC per Model.
Array<MPI_Comm> analysis_comms = parallel_lib.analysis_intra_communicators();
```

These communicators can then be used for initializing parallel simulation instances when registering the plugin interface, where the number of MPI communicators in the array corresponds to one communicator per ParallelConfiguration instance. This is demonstrated below in Derivation.

5.3 Configuring Dakota operation

This section describes several alternate ways to initially set and later manipulate Dakota's configuration, including alternatives to using a text-based input file. The algorithm configuration for a particular Dakota analysis run is managed in its ProblemDescDB, which can be populated via an input file, string literal, or C++ API, and later modified through Dakota's C++ API. All Dakota objects then draw information from this database upon instantiation.

5.3.1 Input data parsing

The simplest way for an application to configure a Dakota analysis problem is to use Dakota's normal input parsing system to populate its problem database (ProblemDescDB). This is done by providing standard Dakota input file syntax through the library interface, via either a file name or string literal. An advantage is that native Dakota syntax can be used, but disadvantages include the requirement for an additional input file beyond those already required by the parent application and that application users also need to know Dakota syntax.

The two ways to configure Dakota via input parsing are shown near the beginning of run_dakota_mixed() in library-_mode.cpp. Here the ProgramOptions are set to either parse from a named file:

```
Dakota::ProgramOptions opts;
opts.input_file(dakota_input_file);
```

or from a string literal provided by the wrapping application:

```
string serial_input = "% Dakota input file ...";
opts.input_string(serial_input);
```

This library approach is coarse-grained in that input is parsed, objects constructed, and the environment is immediately ready to run. The next approaches are more modular.

5.3.2 Problem database insertion

A second approach to configuring Dakota's operation is to bypass parsing phases and directly populate the Problem-DescDB with information on the methods, variables, interface, responses, etc., that define the Dakota analysis problem. This approach requires more interaction with Dakota classes and data structures. However, it can offer usability benefit when the integrating application does not want their users to interact with the full Dakota syntax, or efficiency benefit when for example there are a large number of variables to configure.

In the direct database population approach, Dakota DataMethod, DataModel, DataVariables, DataInterface, and DataResponses objects are instantiated and populated with the desired problem data. These objects are then published to the problem database using insert_nodes() . An example of this approach is available in run_dakota-_data() in library_mode.cpp, where the OPT++ Quasi-Newton method is configured to work on a plugin version of `text_book` or `rosenbrock`. The data objects are populated with their default values upon instantiation and are often sufficient for basic Dakota studies. Only the non-default values need to be specified. Moreover the default Dakota Model is a SingleModel, so this object need not be configured unless tailoring its configuration or using a more advanced model type. Refer to the DataMethod, DataModel, DataVariables, DataInterface, and Data-Responses class documentation and source code for lists of attributes and their defaults. Here is an excerpt of run_dakota_data() that specifies the OPT++ solver after default construction of DataMethod:

```
Dakota::DataMethod   dme;
Dakota::DataMethodRep* dmr = dme.data_rep();
dmr->methodName = Dakota::OPTPP_Q_NEWTON;
```

When using direct database population, it is critical to leave the database in an open, accessible state after initial construction. In this run_dakota_data() example, a flag `check_bcast_construct` is passed into the Library-Environment constructor, indicating that it should not finalize the database and construct Dakota objects. Moreover, it is only necessary to populate the database on rank 0 of the MPI Comm on which Dakota is running. After database objects are inserted or adjusted, the LibraryEnvironment::done_modifying_db() function must be called before proceeding to execute. This synchronizes problem data across all ranks and constructs Dakota objects needed to run the specified analysis.

```
bool check_bcast_construct = false;
Dakota::LibraryEnvironment env(MPI_COMM_WORLD, opts, check_bcast_construct);
if (rank == 0)
  // insert/modify DB, then lock and proceed:
env.done_modifying_db();
env.execute();
```

5.3.3 Mixed mode, callbacks, and late updates

The LibraryEnvironment API also supports mixed approaches that combine the parsing of a Dakota input file (or input string literal) with direct database updates. This approach is motivated by large-scale applications where large vectors are cumbersome to specify in a Dakota input file or where later updates to an input template are needed. The example run_dakota_mixed() in library_mode.cpp demonstrates the combination of these more advanced approaches: (1) input text parsing, (2) database updates via a callback, (3) database updates via direct manipulation, and (4) further runtime updates to the Model before running.

First, a ProgramOptions class is instantiated and configured to parse either an input file or input string literal (as in earlier examples). The passed input data must contain all required inputs so the parser can validate them. Since vector data like variable values/bounds/tags, linear/nonlinear constraint coefficients/bounds, etc., are optional, these potentially large vector specifications can be omitted from the input file and updated later through the database API. Only the variable/response counts necessary for sizing, e.g.:

```
method
  linear_inequality_constraints = 500

variables
  continuous_design = 1000

responses
  objective_functions = 1
  nonlinear_inequality_constraints = 100000
```

and not the lists of values are required in this case. To update or add data after this initial parse, we use the ProblemDescDB::set() family of overloaded functions, e.g.

```
Dakota::RealVector drv(1000, 1.); // vector of length 1000, values initialized to 1.
problem_db.set("variables.continuous_design.initial_point", drv);
```

where the string identifiers are the same identifiers used when pulling information from the database using one of the get_<datatype>() functions (refer to ProblemDescDB for a full list). However, the supported ProblemDescDB::set() options are a restricted subset of the database attributes, focused on vector inputs that can be large scale.

Second, the example demonstrates a user-provided callback function which Dakota will invoke after input parsing to update ProblemDescDB. In `library_mode.cpp`, callback_function() is a user-provided post-parse callback that implements the type Dakota::DbCallbackFunction.

```
static void callback_function(Dakota::ProblemDescDB* db, void *ptr);
```

When Dakota calls this function it will pass back pointers to the ProblemDescDB instance and to user-provided data, so the application may convey its settings by calling methods on the ProblemDescDB, optionally using the provided data. An example of a user data structure is demonstrated in `callback_data`. In this case, when the LibraryEnvironment is constructed, it is constructed with the input data to initially parse, the callback function, and to leave it unlocked for further updates:

```
bool done_with_db = false;
Dakota::LibraryEnvironment env(opts, done_with_db,
      callback_function, &data);
```

Third, the example demonstrates changes to the database after parsing and callback-based updates. Again, these only need happen on Dakota's rank 0 before finalizing the DB with LibraryEnvironment::done_modifying_db(). The example demonstrates:

1. Getting access to the database through `env.problem_description_db()`

2. Setting the database nodes to the appropriate method through `problem_db.resolve_top_method()`

3. Getting data from the DB with a get string array function: `problem_db.get_sa`("interface.application.-analysis_drivers")

4. Setting update data with `problem_db.set`("variables.continuous_design.initial_point", ip);

After any of these three types updates, calling LibraryEnvironment::done_modifying_db() will broadcast any updates (including potentially large vector data and post-process specification data to fill in any vector defaults that have not yet been provided through either file parsing or direct updates. (Note: scalar defaults are handled in the Data class constructors.)

Fourth and finally, run_dakota_mixed() demonstrates modifying a Model's data after database operations and interface plugin are complete. This involves finding the right Model (or other class) instance to modify, and directly adjusting its data through the public API. Since the database is finalized, any updates must be performed through direct set operations on the constructed objects. For example, to update other data such as variable values/bounds/tags or response bounds/targets/tags, refer to the set functions documented in Iterator and Model. As an example, the following code updates the active continuous variable values, which will be employed as the initial guess for certain classes of Iterators:

```
ModelList& all_models  = problem_db.model_list();
Model&     first_model = *all_models.begin();
Dakota::RealVector drv(1000, 1.); // vector of length 1000, values initialized to 1.
first_model.continuous_variables(drv);
```

Remarks

If performing such data updates within the constructor of a DirectApplicInterface extension/derivation (see Creating a simulator plugin interface), then this code is sufficient since the database is unlocked, the active list nodes of the ProblemDescDB have been set for you, and the correct method/model/variables/interface/responses specification instance will get updated. The difficulty in this case stems from the order of instantiation. Since the Variables and Response instances are constructed in the base Model class, prior to construction of Interface instances in derived Model classes, database information related to Variables and Response objects will have already been extracted by the time the Interface constructor is invoked and the database update will not propagate.

Therefore, it is preferred to perform these database set operations at a higher level (e.g., within your main program), prior to allowing Environment to broadcast, construct, and execute, such that instantiation order is not an issue. However, in this case, it is necessary to explicitly manage the list nodes of the ProblemDescDB using a specification instance identifier that corresponds to an identifier from the input file, e.g.:

```
problem_db.set_db_variables_node("MY_VARIABLES_ID");
Dakota::RealVector drv(1000, 1.); // vector of length 1000, values
initialized to 1.
problem_db.set("variables.continuous_design.initial_point", drv);
```

Alternatively, rather than setting just a single data node, all data nodes may be set using a method specification identifier:

```
problem_db.set_db_list_nodes("MY_METHOD_ID");
```

since the method specification is responsible for identifying a model specification, which in turn identifies variables, interface, and responses specifications. If hard-wiring specification identifiers is undesirable, then

```
problem_db.resolve_top_method();
```

can also be used to deduce the active method specification and set all list nodes based on it. This is most appropriate in the case where only single specifications exist for method/model/variables/interface/responses. This is the approach demonstrated in run_dakota_mixed(). In each of these cases, setting list nodes unlocks the corresponding portions of the database, allowing set/get operations.

5.4 Creating a simulator plugin interface

The DirectApplicInterface class provides an interface for Dakota to call the simulation code directly to perform function evaluations mapping variables to responses. This provides the "back end" for Dakota to call back to the simulation framework. Two approaches to defining this direct interface are described here. The first is less common, while the second is recommended when possible.

5.4.1 Extension

The first approach involves extending one of the existing DirectApplicInterface subclasses (TestDriverInterface, MatlabInterface, etc.) to support additional direct simulation interfaces. For example, Dakota algebraic test problems are implemented in TestDriverInterface. One could add additional direct functions to Dakota in TestDriverInterface::derived_map_ac(). In addition, TestDriverInterface::derived_map_if() and TestDriverInterface::derived_map_of() can be extended to perform pre- and post-processing tasks if desired, but this is not required.

While this approach is the simplest, it has the disadvantage that the Dakota library will need to be recompiled when the simulation or its direct interface is modified. If it is desirable to maintain the independence of the Dakota library from the host application, then the derivation approach described in the next section should be employed.

Remarks

If the new direct evaluation function implementation will not be a member function of one of the Dakota classes, then the following prototype should be used in order to pass the required data:

```
int sim(const Dakota::Variables& vars, const Dakota::ActiveSet& set,
Dakota::Response& response);
```

If the new function will be a member function, e.g., in TestDriverInterface, then this can be simplified to

```
int sim();
```

since the data access can be performed through the DirectApplicInterface class attributes.}

5.4.2 Derivation

The second approach is to derive a new interface from DirectApplicInterface and redefine several virtual functions. As demonstrated in SIM::SerialDirectApplicInterface and SIM::ParallelDirectApplicInterface, a typical derived class declaration might be

```
namespace SIM {

class SerialDirectApplicInterface: public Dakota::DirectApplicInterface
{
public:

  // Constructor and destructor

  SerialDirectApplicInterface(const Dakota::ProblemDescDB& problem_db);
  ~SerialDirectApplicInterface();

protected:

  // Virtual function redefinitions

  int derived_map_if(const Dakota::String& if_name);
  int derived_map_ac(const Dakota::String& ac_name);
  int derived_map_of(const Dakota::String& of_name);

private:

  // Data
}

} // namespace SIM
```

where the new derived class resides in the simulation's namespace. Similar to the case of Extension, the DirectApplicInterface::derived_map_ac() function is the required redefinition, and DirectApplicInterface::derived_map_if() and DirectApplicInterface::derived_map_of() are optional.

Typically the new derived_map_ac() implementation delegates to the main simulation application for a function evaluation. Here Dakota variables would get mapped into the simulation's data structures, the simulation executed, and derived response data computed for return to Dakota.

Once a derived application class is created, it must be plugged in, or registered, with the appropriate Interface in the LibraryEnvironment. In MPI cases where Dakota is potentially managing concurrent evaluations of the simulation, the plugin must be configured to run on the right MPI sub-communicator, or Dakota analysis_comm. The simpler case is demonstrated in serial_interface_plugin() in library_mode.cpp, while a more advanced case using the analysis communicator is shown in parallel_interface_plugin().

The Dakota LibraryEnvironment provides a convenience function to plugin an Interface. This example will replace any interface found matching the given model, interface, and analysis driver with the passed plugin interface:

```
std::string model_type(""); // demo: empty string will match any model type
std::string interf_type("direct");
std::string an_driver("plugin_rosenbrock");

Dakota::ProblemDescDB& problem_db = env.problem_description_db();
std::shared_ptr<Dakota::Interface> serial_iface =
  std::make_shared<SIM::SerialDirectApplicInterface>(problem_db);

bool plugged_in =
  env.plugin_interface(model_type, interf_type, an_driver, serial_iface);
```

The LibraryEnvironment also provides convenience functions that allow the client to iterate the lists of available interfaces or models for more advanced cases. For instance if the client knows there is only a single interface active, it could get the list of available interfaces of length 1 and plugin to the first one. In the more advanced case where the simulation interface instance should manage parallel simulations within the context of an MPI communicator, one should pass in the relevant analysis communicator(s) to the derived constructor. For the latter case of looping over a set of models, the simplest approach of passing a single analysis communicator would use code similar to

```
Dakota::ModelList filt_models =
  env.filtered_model_list("single", "direct", "plugin_text_book");

Dakota::ProblemDescDB& problem_db = env.problem_description_db();
Dakota::ModelLIter ml_iter;
for (ml_iter = filt_models.begin(); ml_iter != filt_models.end(); ++ml_iter) {
  // set DB nodes to input specification for this Model
  problem_db.set_db_model_nodes(ml_iter->model_id());

  Dakota::Interface& model_interface = ml_iter->derived_interface();

  // Parallel case: plug in derived Interface object with an analysisComm.
  // Note: retrieval and passing of analysisComm is necessary only if
  // parallel operations will be performed in the derived constructor.

  // retrieve the currently active analysisComm from the Model.  In the most
  // general case, need an array of Comms to cover all Model configurations.
  const MPI_Comm& analysis_comm = ml_iter->analysis_comm();

  // don't increment ref count since no other envelope shares this letter
  model_interface.assign_rep(new
    SIM::ParallelDirectApplicInterface(problem_db, analysis_comm), false)
      ;
}
```

The file library_mode.cpp demonstrates each of these approaches. Since a Model may be used in multiple parallel contexts and may therefore have a set of parallel configurations, a more general approach would extract and pass an array of analysis communicators to allow initialization for each of the parallel configurations.

New derived direct interface instances inherit various attributes of use in configuring the simulation. In particular, the ApplicationInterface::parallelLib reference provides access to MPI communicator data (e.g., the analysis communicators discussed above), DirectApplicInterface::analysisDrivers provides the analysis driver names specified by the user in the input file, and DirectApplicInterface::analysisComponents provides additional analysis component identifiers (such as mesh file names) provided by the user which can be used to distinguish different instances of the same simulation interface. It is worth noting that inherited attributes that are set as part of the parallel configuration (instead of being extracted from the ProblemDescDB) will be set to their defaults following construction of the base class instance for the derived class plug-in. It is not until run-time (i.e., within derived_map_if/derived_map_ac/derived_map_of) that the parallel configuration settings are re-propagated to the plug-in instance. This is the reason that the analysis communicator should be passed in to the constructor of a parallel plug-in, if the constructor will be responsible for parallel application initialization.

5.5 Retrieving data after a run

After executing the Dakota Environment, final results can be obtained through the use of Environment::variables_-results() and Environment::response_results(), e.g.:

```
// retrieve the final parameter values
const Variables& vars = env.variables_results();

// retrieve the final response values
const Response& resp  = env.response_results();
```

In the case of optimization, the final design is returned, and in the case of uncertainty quantification, the final statistics are returned. Dakota has a prototype results database, which will eventually provide better access to the results from a study.

5.6 Linking against the Dakota library

This section presumes Dakota has been configured with CMake, compiled, and installed to a `CMAKE_INSTALL_-PREFIX` using `make install` or equivalent. The Dakota libraries against which you must link will typically install to `CMAKE_INSTALL_PREFIX/bin/` and `CMAKE_INSTALL_PREFIX/lib/`, while headers are provided in `CMAKE_INSTALL_PREFIX/lib/`. The core Dakota C and C++ code is in the library `dakota_src`, while Fortran code lives in the `dakota_src_fortran` library. Runtime libraries for any configure-enabled Dakota third-party software components (such as DOT, NPSOL, OPT++, LHS, etc.) are also installed to the lib/ directory. Applications link against these Dakota libraries by specifying appropriate include and link directives.

There two primary ways to determine the necessary Dakota-related libraries and link order for linking your application. First, when running CMake, a list of required Dakota and Dakota-included third-party libraries will be output to the console, e.g.,

```
-- Dakota_LIBRARIES: dakota_src;dakota_src_fortran;nidr;teuchos;pecos;pecos_src;lhs;mods;mod;dfftpack;sparsegr
```

While external dependencies will be output as:

```
-- Dakota_TPL_LIBRARIES: /usr/lib64/libcurl.so;/usr/lib64/openmpi/lib/libmpi_cxx.so;debug;/usr/lib64/libz.so;d
```

Note that depending on how you configured Dakota, some libraries may be omitted from these lists (for example commercial add-ons NPSOL, DOT, and NLPQL), or additional libraries may appear.

A second option is to check which libraries appear in `CMAKE_INSTALL_PREFIX/bin/` `CMAKE_INSTALL-_PREFIX/lib/`, or more accurately, see the file Makefile.export.Dakota in the Dakota build/src/ or installation include/ directory. Here are some additional notes on specific libraries:

- Some Boost libraries (`boost_regex`, `boost_filesystem`, `boost_system`, `boost_serialization`) are required, and other Boost library components may be required depending on configuration, e.g., `boost-_signals` when configuring with `HAVE_ACRO:BOOL=TRUE`
- System compiler and math libraries may need to be included, as may additional system libraries such as Expat and Curl, depending on how Dakota is configured.
- If configuring with graphics, you will need to add the `dakota_sciplot` library and system X libraries (partial list here):

  ```
  -lXpm -lXm -lXt -lXmu -lXp -lXext -lX11 -lSM -lICE
  ```

- When configuring with AMPL (`HAVE_AMPL:BOOL=ON`), the AMPL solver library may require `dl`, `funcadd0.o` and `fl` libraries. We have experienced problems with the creation of `libamplsolver.a` on some platforms; use the dakota-users mailing list to get help with any problems related to this.
- Optional library GSL (discouraged due to GPL license) and if linking with system-provided GSL, `gslcblas` may be needed if Dakota was configured with them.

- Newmat: as of Dakota 5.2, `-lnewmat` is no longer required

Finally, it is important to use the same C++ compiler (possibly an MPI wrapper) for compiling Dakota and your application and potentially include Dakota-related preprocessor defines as emitted by CMake during compilation of Dakota and included in Makefile.export.Dakota. This ensures that the platform configuration settings are properly synchronized across Dakota and your application.

Chapter 6

Performing Function Evaluations

Performing function evaluations is one of the most critical functions of the Dakota software. It can also be one of the most complicated, as a variety of scheduling approaches and parallelism levels are supported. This complexity manifests itself in the code through a series of cascaded member functions, from the top level model evaluation functions, through various scheduling routines, to the low level details of performing a system call, fork, or direct function invocation. This section provides an overview of the primary classes and member functions involved.

6.1 Synchronous function evaluations

For a synchronous (i.e., blocking) mapping of parameters to responses, an iterator invokes Model::evaluate() to perform a function evaluation. This function is all that is seen from the iterator level, as underlying complexities are isolated. The binding of this top level function with lower level functions is as follows:

- Model::evaluate() utilizes Model::derived_evaluate() for portions of the response computation specific to derived model classes.
- Model::derived_evaluate() directly or indirectly invokes Interface::map().
- Interface::map() utilizes ApplicationInterface::derived_map() for portions of the mapping specific to derived application interface classes.

6.2 Asynchronous function evaluations

For an asynchronous (i.e., nonblocking) mapping of parameters to responses, an iterator invokes Model::evaluate_nowait() multiple times to queue asynchronous jobs and then invokes either Model::synchronize() or Model::synchronize_nowait() to schedule the queued jobs in blocking or nonblocking fashion. Again, these functions are all that is seen from the iterator level, as underlying complexities are isolated. The binding of these top level functions with lower level functions is as follows:

- Model::evaluate_nowait() utilizes Model::derived_evaluate_nowait() for portions of the response computation specific to derived model classes.
- This derived model class function directly or indirectly invokes Interface::map() in asynchronous mode, which adds the job to a scheduling queue.
- Model::synchronize() or Model::synchronize_nowait() utilize Model::derived_synchronize() or Model::derived_synchronize_nowait() for portions of the scheduling process specific to derived model classes.
- These derived model class functions directly or indirectly invoke Interface::synchronize() or Interface::synchronize_nowait().

- For application interfaces, these interface synchronization functions are responsible for performing evaluation scheduling in one of the following modes: master dynamic, peer dynamic or peer static.
- *NOTE: The Interface evaluation scheduling in Dakota was refactored for releases 5.4 and 6.0. Discussion of the new Interface-related functions is currently missing here.*

6.3 Analyses within each function evaluation

NOTE: The Interface evaluation scheduling in Dakota was refactored for releases 5.4 and 6.0. Discussion of the new Interface-related functions for analyses is currently missing here.

The discussion above covers the parallelism level of concurrent function evaluations serving an iterator. For the parallelism level of concurrent analyses serving a function evaluation, similar schedulers are involved

to support synchronous local, asynchronous local, message passing, and hybrid modes. Not all of the schedulers are elevated to the ApplicationInterface level since the system call and direct function interfaces do not yet support nonblocking local analyses (and therefore support synchronous local and message passing modes, but not asynchronous local or hybrid modes). Fork interfaces, however, support all modes of analysis parallelism.

Chapter 7

Working with Variable Containers and Views

Variable views control the subset of variable types that are active and inactive within a particular iterative study. For design optimization and uncertainty quantification (UQ), for example, the active variables view consists of design or uncertain types, respectively, and any other variable types are carried along invisible to the iterative algorithm being employed. For parameter studies and design of experiments, however, a variable subset view is not imposed and all variables are active. Selected UQ methods can also be toggled into an "All" view using the `active all` variables input specification. When not in an All view, finer gradations within the uncertain variable sets are also relevant: probabilistic methods (reliability, stochastic expansion) view aleatory uncertain variables as active, nonprobabilistic methods (interval, evidence) view epistemic uncertain variables as active, and a few UQ methods (sampling) view both as active. In a more advanced NestedModel use case such as optimization under uncertainty, design variables are active in the outer optimization context and the uncertain variables are active in the inner UQ context, with an additional requirement on the inner UQ level to return derivatives with respect to its "inactive" variables (i.e., the design variables) for use in the outer optimization loop.

For efficiency, contiguous arrays of data store variable information for each of the domain types (continuous, discrete integer, and discrete real), but active and inactive views into them permit selecting subsets in a given context. This management is encapsulated into the Variables and SharedVariablesData classes. This page clarifies concepts of relaxed (formerly merged) vs. mixed, fine-grained vs. aggregated types, domain types, and views into contiguous arrays.

We begin with an overview of the storage and management concept, for which the following two sections describe the storage of variable values and meta-data about their organization, used in part to manage views. They are intended to communicate rationale to maintainers of Variables and SharedVariablesData classes. The final section provides a discussion of active and inactive views.

7.1 Storage in Variables

As described in the Main Page Variables, a Variables object manages variable types (design, aleatory uncertain, epistemic uncertain, and state) and domain types (continuous, discrete integer, and discrete real) and supports different approaches to either distinguishing among these types or aggregating them. Two techniques are used in cooperation to accomplish this management: (1) class specialization (RelaxedVariables or MixedVariables) and (2) views into contiguous variable arrays. The latter technique is used whenever it can satisfy the requirement, with fallback to class specialization when it cannot. In particular, aggregation or separation of variable types can be accomplished with views, but for aggregation or separation of variable domains, we must resort to class specialization in order to relax discrete domain types. In this class specialization, a RelaxedVariables object combines continuous and discrete types (relaxing integers to reals) whereas a MixedVariables object maintains the integer/real distinction throughout.

The core data for a Variables instance is stored in a set of three continguous arrays, corresponding to the domain types: allContinuousVars, allDiscreteIntVars, and allDiscreteRealVars, unique to each Variables instance.

Within the core variable data arrays, data corresponding to different aggregated variable types are stored in sequence for each domain type:

- continuous: [design, aleatory uncertain, epistemic uncertain, state]
- discrete integer: [design, aleatory uncertain, (epistemic uncertain), state]
- discrete real: [design, aleatory uncertain, (epistemic uncertain), state]

Note there are currently no epistemic discrete variables. This domain type ordering (continuous, discrete integer, discrete real) and aggregated variable type ordering (design, aleatory uncertain, epistemic uncertain, state) is preserved whenever distinct types are flattened into single contiguous arrays. Note that the aleatory and epistemic uncertain variables contain sub-types for different distributions (e.g., normal, uniform, histogram, poisson), and discrete integer types include both integer ranges and integer set sub-types. All sub-types are ordered according to their order of appearance in dakota.input.nspec.

When relaxing in MixedVariables, the allContinuousVars will also aggregate the discrete types, such that they contain ALL design, then ALL uncertain, then ALL state variables, each in aggregated type order; the allDiscreteIntVars and allDiscreteRealVars arrays are empty.

7.2 Storage in SharedVariablesData

Each Variables instance contains a reference-counted SharedVariablesData object that stores information on the variables configuration. This configuration data includes counts, types, IDs, and labels, which are often the same across many Variables instances. Thus, SharedVariablesData is intended to reduce the memory footprint by allowing the sharing of a single copy of redundant information among different Variables instances.

One of the purposes of this shared information is to support mappings between variable types, IDs, and indices into the storage arrays. Variable "types" refer to the fine-grained variable types a user would specify in an input file, as enumerated in DataVariables.hpp, e.g, CONTINUOUS_DESIGN, WEIBULL_UNCERTAIN, DISCRETE_STATE_R-ANGE, etc. variablesComponents is a map from these variable types to counts of how many are present.

In contrast, the variablesCompsTotals array stores total counts of each "aggregated type" (design, aleatory uncertain, epistemic uncertain, state) which might be selected to be active in a given view. Thus this array has length 12 to track the combinations of three domain type storage arrays with four possible aggregated variable types: {continuous, discrete integer, discrete real} x {design, aleatory uncertain, epistemic uncertain, state}. For example, the first entry of this array stores the number of continuous design variables, the second the number of discrete integer design (including both discrete design range and discrete design set integer types), and the last the number of discrete real state variables.

The arrays allContinuousTypes, allDiscreteIntTypes, and allDiscreteRealTypes are sized to match the corresponding core domain type storage arrays. They track the fine-grained variable type stored in that entry of the data array (since when relaxed, the continuous array may be storing data corresponding to discrete data).

Finally allContinuousIds stores the 1-based IDs of the variables stored in the allContinuousVars array, i.e., the variable number of all the problem variables considered as a single contiguous set, in aggregate type order. For relaxed (formerly merged) views, relaxedDiscreteIds stores the 1-based IDs of the variables which have been relaxed into the continuous array.

These counts, types, and IDs are most commonly used within the Model classes for mappings between variables objects at different levels of a model recursion. See, for example, the variable mappings in the NestedModel constructor.

7.3 Active and inactive views

The pair SharedVariablesDataRep::variablesView tracks the active and inactive views of the data, with values taken from the enum in DataVariables.hpp. The valid values include EMPTY and the combinations {relaxed, mixed} x {all, design, aleatory uncertain, epistemic uncertain, uncertain, state}. The ALL cases indicate aggregation of the design, aleatory uncertain, epistemic uncertain, and state types, whereas the DISTINCT cases indicate either no aggregation (design, aleatory uncertain, epistemic uncertain, state) or reduced aggregation (aleatory+epistemic uncertain). The active view is determined by the algorithm in use, managed in Variables::get_view(). Any inactive view is set based on higher level iteration within a model recursion (e.g., a NestedModel), which enables lower level iteration to return derivatives with respect to variables that are active at the higher level. In the case where there is no higher level iteration, then the inactive view will remain EMPTY. It is important to stress that "inactive" at one level corresponds to active at another, and therefore the inactive set of variables should not be interpreted as the strict complement of the active set of variables; rather, active and inactive are both subsets whose union may still be a subset of the total container (more precise terminology might involve "primary" active and "secondary" active or similar). An active complement view could potentially be supported in the future, should the need arise, although this view would require management of non-contiguous portions of the aggregated arrays.

Given these groupings (views), the active and inactive subsets of the allContinuousVars, allDiscreteIntVars, and all-DiscreteRealVars arrays are always contiguous, permitting vector views of the underlying data using either Teuchos-::View (for numerical vectors) or Boost.MultiArray (for book-keeping arrays) views.

When a Variables envelope is constructed, its letter is initialized to either a RelaxedVariables or MixedVariables object depending on the active view. The derived classes size the contiguous storage arrays to accomodate all the problem variables, and then initialize active views into them, which could involve either subsets (DISTINC-T active views) or views of the full arrays (ALL active views). Inactive views, on the other hand, are initialized during construction of a model recursion (e.g., a call to Model::inactive_view() in the NestedModel constructor). Thus, active variable subsets are always available but inactive variable subsets will be EMPTY prior to them being initialized within a Model recursion.

Accessors for continuous variables include:

- continuous_variables(): returns the active view which might return all (ALL views) or a subset (DISTINCT views) such as design, uncertain, only aleatory uncertain, etc.
- inactive_continuous_variables(): returns the inactive view which which is either a subset or empty
- all_continuous_variables(): returns the full vector allContinuousVars

and this pattern is followed for active/inactive/all access to discrete_int_variables() and discrete_real_variables() as well as for labels, IDs, and types in SharedVariablesData and variable bounds in Constraints.

Chapter 8

Demo TPL

This is a simple *Demo* which serves as a working example for bringing a new Third-Party Library (TPL) into Dakota. The *Demo* will serve to show minimal requirements for:

- building and running the *Demo*
- building a TPL under Dakota using CMake
- exposing TPL functionality to Dakota
- exposing TPL options through Dakota
- transferring data between a TPL and Dakota

Following this *Demo*, a developer should be able to integrate an optimization TPL/method that:

- is derivative-free
- operates over continuous variables
- supports any of the following types of constraints
  - bound constraints
  - nonlinear inequality constraints
  - nonlinear equality constraints

Quickstart: Building and Running the *Demo*

In order to build and run this *Demo*, it is necessary to build Dakota from source. Complete instructions for doing so can be found at `https://dakota.sandia.gov/content/build-compile-source-code`. At the point in the instructions where cmake is invoked, append `-DHAVE_DEMO_TPL:BOOL=ON` to the cmake invocation.

Building Dakota with the *Demo* TPL enabled will also activate a working example found in `$DAKOTA_BUILD/test/dakota_demo_app`, where `$DAKOTA_BUILD` is the root of the Dakota build tree. The test can be run from `$DAKOTA_BUILD/test` using

```
`ctest -R demo_app`
```

Summary info will be output to the screen, and test artifacts can be found in `$DAKOTA_BUILD/test/dakota_demo_app`.

Alternatively the example can be run in the same way a user runs Dakota. In particular, from the $DAKOTA_BUILD/test/dakota_demo_app directory, issue the following command:

```
`/path/to/dakota -i dakota_demo_app.in`
```

The remainder of this file describes how to integrate a TPL into Dakota using the *Demo* (found in `$DAKOTA_SRC/packages/external/demo_tpl`) as an example.

Building a TPL under Dakota using Cmake

This section shows how to include the relevant parts of the *Demo* TPL as a library that Dakota builds and includes as part of its own native Cmake build.

Assuming the *Demo* tpl source code has been placed alongside other Dakota TPLs in `$DAKOTA_SRC/packages/external/demo_tpl`, a simple *CMakeLists.txt* file can be created at this location to allow Dakota to include it within its own Cmake setup. An minimal example might include:

```
# File $DAKOTA_SRC/packages/external/demo_tpl/CMakeLists.txt

cmake_minimum_required(VERSION 2.8)
project("DEMO_TPL" CXX)
SUBDIRS(src)
```

In the src subdirectory of demo_tpl would be another *CMakeLists.txt* file which essentially identifies the relevant source code to be compiled into a library along with defining the library which Daktoa will later include, e.g.

```
# File $DAKOTA_SRC/packages/external/demo_tpl/src/CMakeLists.txt

set(demo_tpl_HEADERS
    demo_opt.hpp
   )

set(demo_tpl_SOURCES
    demo_opt.cpp
   )

# Set the DEMO_TPL library name.
add_library(demo_tpl ${demo_tpl_SOURCES})

# Define install targets for "make install"
install(TARGETS demo_tpl EXPORT ${ExportTarget} DESTINATION lib)
```

Note that it is possible to use Cmake's glob feature to bring in all source and header files, but care must be taken to avoid introducing `main(...)` symbols which will collide with Dakota's `main` at link time.

At this point, Dakota's *CMakeLists.txt* files will need to be modified to include the *Demo* TPL. The following modifications can be used to bring in the *Demo* TPL, conditioned on having `-DHAVE_DEMO_TPL:BOOL=ON` defined when invoking cmake to configure Dakota:

```
# File $DAKOTA_SRC/packages/CMakeLists.txt

<... snip ...>
  option(HAVE_DEMO_TPL "Build the Demo_TPL package." OFF)
<... end snip ...>

<... snip ...>
  if(HAVE_DEMO_TPL)
    add_subdirectory(external/demo_tpl)
  endif(HAVE_DEMO_TPL)
<... end snip ...>
```

This next modification to Dakota will allow the *Demo* TPL to be used by other Dakota source code by including the necessary include paths, link-time libraries and needed #defines:

```
# File $DAKOTA_SRC/src/CMakeLists.txt

<... snip ...>

if(HAVE_DEMO_TPL)
  set(DAKOTA_DEMOTPL_ROOT_DIR "${Dakota_SOURCE_DIR}/packages/external/demo_tpl")
  list(APPEND DAKOTA_INCDIRS
      ${DAKOTA_DEMOTPL_ROOT_DIR}/dakota_src
      ${DAKOTA_DEMOTPL_ROOT_DIR}/src)
set(iterator_src ${iterator_src} ${Dakota_SOURCE_DIR}/packages/external/demo_tpl/dakota_src/DemoOptimizer.
      cpp)
  list(APPEND DAKOTA_PKG_LIBS demo_tpl)
list(APPEND EXPORT_TARGETS demo_tpl)
  add_definitions("-DHAVE_DEMO_TPL")
endif(HAVE_DEMO_TPL)

<... end snip ...>
```

Test-Driven Code Development

Before making concrete changes, it is often helpful to create a simple Dakota test which will serve to guide the process. This is akin to test-driven development which essentially creates a test which fails until everything has been implemented to allow it to run and pass. A candidate test for the current activity could be the following:

```
# File $DAKOTA_SRC/test/dakota_demo_app.in

    method,
        demo_tpl
        options_file = "demo_tpl.opts"

    variables,
        continuous_design = 3
        initial_point      -1.0     1.5    2.0
        upper_bounds       10.0    10.0   10.0
        lower_bounds       -10.0  -10.0  -10.0
        descriptors         'x1'   'x2'   'x3'

    interface,
        direct
        analysis_driver = 'text_book'

    responses,
        objective_functions = 1
        no_gradients
        no_hessians
```

For this test to run, we will need to be able to pass parsed options to the *Demo* TPL and exchange parameters and response values between Dakota and *Demo* TPL. These details are presented in the following sections.

Exposing TPL Functionality to Dakota

Dakota performs some internal checks in order to confirm applicability of a specified method to the problem defined. In order for Dakota to perform those checks for the *Demo* TPL, the functionality of the method must be communicated to Dakota. That is done via implementation of a traits class. Traits define the types of problems and data formats the *Demo* TPL supports by overriding the default traits accessors in TraitsBase. By default, nothing is supported, and the TPL integrator must explicitly turn on the traits for any supported features.

```
// File $DAKOTA_SRC/packages/external/demo_tpl/dakota_src/DemoOptimizer.hpp

class DemoOptTraits: public TraitsBase
{
public:
  <... snip ...>
  //
  //- Heading: Constructor and destructor
  //

  DemoOptTraits() { }

  virtual ~DemoOptTraits() { }
  <... end snip ...>

  <... snip ...>
  //
  //- Heading: Virtual member function redefinitions
  //

  bool supports_continuous_variables() override
    { return true; }
  <... end snip ...>
}; // class DemoOptTraits
```

A complete list of traits can be found in `$DAKOTA_SRC/src/DakotaTraitsBase.hpp`. The subset applicable to the *Demo* TPL can be found in `$DAKOTA_SRC/packages/external/demo_tpl/dakota_src/DemoOptimizer.hpp`.

Exposing TPL Options Through Dakota

The simplest way to pass options to a TPL is via a file. The *Demo* TPL has the ability to read in a file of method options when given a file name. This file name can be specified in the Dakota input file and retrieved as illustrated below.

```
// File $DAKOTA_SRC/packages/external/demo_tpl/dakota_src/DemoOptimizer.cpp

  <... snip ...>
  // Check for native Demo_Opt input file.  The file name needs to be
  // included in the Dakota input file.
  String adv_opts_file = probDescDB.get_string("method.advanced_options_file");
  if (!adv_opts_file.empty())
  {
    if (!boost::filesystem::exists(adv_opts_file))
    {
      Cerr << "\nError: Demo_Opt options_file '" << adv_opts_file
           << "' specified, but file not found.\n";
      abort_handler(METHOD_ERROR);
    }
  }
  <... end snip ...>
```

If desired, common stopping criteria can be retrieved from the Dakota input file, rather than passed through a TPL-specific input file, as follows.

```
// File $DAKOTA_SRC/packages/external/demo_tpl/dakota_src/DemoOptimizer.cpp

  <... snip ...>
  get_common_stopping_criteria(max_fn_evals, max_iters, conv_tol,
  min_var_chg, obj_target );
  <... end snip ...>
```

Exchanging Parameters and Reponses

Like any TPL, the *Demo* TPL will need to exchange parameter and obective function values with Dakota. For purposes of demonstration, an example interface between Dakota and the *Demo* TPL can be seen in `$DAKOTA_SRC/packages/external/demo_tpl/dakota_src/DemoOptimizer.hpp` (with corresponding .cpp in the same directory). Within these files is a key callback interface used by the *Demo* TPL to obtain objective function values for given parameter values (3 in the test above), eg:

```
// File $DAKOTA_SRC/packages/external/demo_tpl/dakota_src/DemoOptimizer.cpp

Real
DemoTPLOptimizer::compute_obj(const std::vector<double> & x, bool verbose)
{
  // Tell Dakota what variable values to use for the function
  // valuation.  x must be (converted to) a std::vector<double> to use
  // this demo with minimal changes.
  set_variables<>(x, iteratedModel, iteratedModel.current_variables());

  // Evaluate the function at the specified x.
  iteratedModel.evaluate();

  // Retrieve the the function value and sign it appropriately based
  // on whether minimize or maximize has been specified in the Dakota
  // input file.
  double f = dataTransferHandler->get_response_value_from_dakota(iteratedModel.current_response());

  return f;
}
```

In this instance, the *Demo* TPL uses `std::vector<double>` as its native parameter vector data type and is calling back to the example problem (Dakota model) via an interface to Dakota to obtain a single `double` (aliased to `Real` in Dakota) obective function value for a given set of parameter values. These data exchanges are facilitated by used of "data adapters" supplied by Dakota with the `set_variables<>(...)` utility and `dataTransferHandler` helper class utilized in this case.

For problems involving nonlinear equality and inequality constraints Dakota treats these as additional responses to the objective funtction(s). The *Demo* TPL supports both types for purposes of showing how these additional responses can be computed by Dakota (via interface to an underlying model) and transferred to the TPL. Similar to the call (by *Demo*) to `compute_obj(...)` are two additional methods to compute and transfer nonlinear constraint responses, eg:

```
// File $DAKOTA_SRC/packages/external/demo_tpl/dakota_src/DemoOptimizer.cpp
```

```
void
DemoTPLOptimizer::compute_nln_eq(std::vector<Real> &c, const std::vector<Real> &x, bool verbose)
{
  // Tell Dakota what variable values to use for the nonlinear constraint
  // evaluations.  x must be (converted to) a std::vector<double> to use
  // this demo with minimal changes.
  set_variables<>(x, iteratedModel, iteratedModel.current_variables());

  // Evaluate the function at the specified x.
  iteratedModel.evaluate();

  // Use an adapter to copy data
  dataTransferHandler->get_nonlinear_eq_constraints_from_dakota(iteratedModel.current_response(), c);
}

void
DemoTPLOptimizer::compute_nln_ineq(std::vector<Real> &c, const std::vector<Real> &x, bool verbose)
{
  set_variables<>(x, iteratedModel, iteratedModel.current_variables());
  iteratedModel.evaluate();
  dataTransferHandler->get_nonlinear_ineq_constraints_from_dakota(iteratedModel.current_response(), c);
}
```

Both of these callback methods (to Dakota), `compute_nln_eq(...)` and `compute_nln_ineq(...)` follow the same pattern as seen for the objective function callback: 1) set the Dakota model with the current variables (parameters), 2) evaluate the model and 3) transfer the desired response (objective or constraint) back to the TPL. The third step is facilitated by the appropriate call to the `dataTransferHandler` helper class. It should be noted that even though as many as three separate calls to evaluate the model are made for the same parameter values, Dakota maintains an internal cache of response values for each unique set. The model will be evaluated the first time a new set of parameter values is provided, but the cached values will simply be returned thereafter, thereby avoiding superfluous model evaluations.

Dakota must also provide initial parameter values to the *Demo* TPL and retrieve final objective function and variable values from the *Demo* TPL. The initial values for parameters and bound constraints can be obtained from Dakota with the `get_variables<>(...)` helpers. This example returns the values to a standard vector of doubles (Reals). These values can then be passed to the *Demo* TPL using whatever API is provided. The API for this last step varies with the particular TPL, and *Demo* provides a function `set_problem_data` in this case.

```
// File $DAKOTA_SRC/packages/external/demo_tpl/dakota_src/DemoOptimizer.cpp

void DemoTPLOptimizer::initialize_variables_and_constraints()
{
  // Get the number of variables, the initial values, and the values
  // of bound constraints.  They are returned to standard C++ data
  // types.  This example considers only continuous variables.  Other
  // types of variables and constraints will be added at a later time.
  // Note that double is aliased to Real in Dakota.
  int num_total_vars = numContinuousVars;
  std::vector<Real> init_point(num_total_vars);
  std::vector<Real> lower(num_total_vars),
                    upper(num_total_vars);

  // More on DemoOptTraits can be found in DemoOptimizer.hpp.
  get_variables(iteratedModel, init_point);
  get_variable_bounds_from_dakota<DemoOptTraits>( lower, upper );

  // Replace this line by whatever the TPL being integrated uses to
  // ingest variable values and bounds, including any data type
  // conversion needed.

  // ------------------  TPL_SPECIFIC  ------------------
  demoOpt->set_problem_data(init_point,   //  "Initial Guess"
                            lower     ,   //  "Lower Bounds"
                            upper      ); //  "Upper Bounds"

}
```

The TPL should be able to return an optimal objective function value and the corresponding variable (parameter) values via its API. As has been the case throughout, the data should be doubles (aliased to Real in Dakota). The following code takes the values returned by *Demo* via a call to `get_best_f()` and sets the Dakota data structures that contain final objective and variable values. It adjusts the sign of the objective based on whether minimize or maximize has been specified in the Dakota input file (minimize is the default). If the problem being optimized involves nonlinear equality and/or inequality constraints, these will also need to be obtained from the TPL and passed to Dakota as part of the array of best function values (responses).

```
// File $DAKOTA_SRC/packages/external/demo_tpl/dakota_src/DemoOptimizer.cpp
// in method void DemoTPLOptimizer::core_run()

  // Replace this line with however the TPL being incorporated returns
  // the optimal function value.  To use this demo with minimal
  // changes, the returned value needs to be (converted to) a
  // double.
  double best_f = demoOpt->get_best_f(); // TPL_SPECIFIC

  // If the TPL defaults to doing minimization, no need to do
  // anything with this code.  It manages needed sign changes
  // depending on whether minimize or maximize has been specified in
  // the Dakota input file.
  const BoolDeque& max_sense = iteratedModel.primary_response_fn_sense();
  RealVector best_fns(iteratedModel.response_size()); // includes nonlinear contraints

  // Get best (single) objcetive value respecting max/min expectations
  best_fns[0] = (!max_sense.empty() && max_sense[0]) ?  -best_f : best_f;

  // Get best Nonlinear Equality Constraints from TPL
  if( numNonlinearEqConstraints > 0 )
  {
    auto best_nln_eqs = demoOpt->get_best_nln_eqs(); // TPL_SPECIFIC
    dataTransferHandler->get_best_nonlinear_eq_constraints_from_tpl(
                                        best_nln_eqs,
                                        best_fns);
  }

  // Get best Nonlinear Inequality Constraints from TPL
  if( numNonlinearIneqConstraints > 0 )
  {
    auto best_nln_ineqs = demoOpt->get_best_nln_ineqs(); // TPL_SPECIFIC

    dataTransferHandler->get_best_nonlinear_ineq_constraints_from_tpl(
                                        best_nln_ineqs,
                                        best_fns);
  }

  bestResponseArray.front().function_values(best_fns);

  std::vector<double> best_x = demoOpt->get_best_x(); // TPL_SPECIFIC

  // Set Dakota optimal value data.
  set_variables<>(best_x, iteratedModel, bestVariablesArray.front());
```

Member SurfpackApproximation::build () override

Right now, we're completely deleting the old data and then recopying the current data into a SurfData object. This was just the easiest way to arrive at a solution that would build and run. This function is frequently called from addPoint rebuild, however, and it's not good to go through this whole process every time one more data point is added.

Member SurfpackApproximation::hessian (const RealVector &c_vars) override

Make this acceptably efficient

Member SurfpackApproximation::hessian (const Variables &vars) override

Make this acceptably efficient

Chapter 9

Namespace Index

9.1 Namespace List

Here is a list of all documented namespaces with brief descriptions:

Chapter 10

Hierarchical Index

10.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

Chapter 11

Class Index

11.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 12

File Index

12.1 File List

Here is a list of all documented files with brief descriptions:

Chapter 13

Namespace Documentation

13.1 dakota Namespace Reference

dakota (lowercase) namespace for new Dakota modules

Namespaces

- surrogates

  namespace for new Dakota surrogates module
- util

  namespace for new Dakota utilities module

Typedefs

- using RowVectorXd = Eigen::RowVectorXd

  Eigen generic row vector of doubles in Dakota namespace.
- using VectorXd = Eigen::VectorXd

  Eigen generic column vector of doubles in Dakota namespace.
- using MatrixXd = Eigen::MatrixXd

  Eigen generic matrix of doubles in Dakota namespace.
- using VectorXi = Eigen::VectorXi

  Eigen generic vector of integers in Dakota namespace.
- using MatrixXi = Eigen::MatrixXi

  Eigen generic matrix of integers in Dakota namespace.
- using Real = double

  Dakota real floating point type.
- using RealMatrix = Teuchos::SerialDenseMatrix< int, Real >

  Dakota matrix of reals.
- using RealVector = Teuchos::SerialDenseVector< int, Real >

  Dakota vector of reals.
- using ParameterList = Teuchos::ParameterList

  Teuchos ParameterList for options management in Dakota namespace.
- using StringArray = std::vector< std::string >

  Array of strings.

Functions

- template<typename... Ts>
  void silence_unused_args (const Ts...)

  silence unused parameter warning; use to indicate those parameters are intentionally unused

Variables

- const double near_zero = std::abs(10.0 ∗ std::numeric_limits<double>::min())

  Double precision difference tolerance.

13.1.1 Detailed Description

dakota (lowercase) namespace for new Dakota modules

13.2 Dakota Namespace Reference

The primary namespace for DAKOTA.

Classes

- class ActiveSubspaceModel

  Active subspace model for input (variable space) reduction.
- class AdaptedBasisModel

  Adapted basis model for input (variable space) reduction.
- class AdapterModel

  Derived model class which wraps call-back functions for solving minimization sub-problems.
- class ApplicationInterface

  Derived class within the interface class hierarchy for supporting interfaces to simulation codes.
- class ApproximationInterface

  Derived class within the interface class hierarchy for supporting approximations to simulation-based results.
- class APPSEvalMgr

  Evaluation manager class for APPSPACK.
- class AppsTraits

  HOPSPACK-specific traits class.
- class APPSOptimizer

  Wrapper class for HOPSPACK.
- class BootstrapSamplerBase

  Base class/interface for the bootstrap sampler.
- class BootstrapSampler

  Actual boostrap sampler implementation for common data types.
- class BootstrapSampler< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > >

  Bootstrap sampler that is specialized to allow for the boostrapping of RealMatrix.
- class BootstrapSamplerWithGS

  A derived sampler to allow for user specification of the accessor methods.
- class C3Approximation

  Derived approximation class for global basis polynomials.
- class C3FnTrainData

  Handle for reference-counted pointer to C3FnTrainDataRep body.

- class COLINApplication
- class COLINTraits

  A version of TraitsBase specialized for COLIN optimizers.
- class COLINOptimizer

  Wrapper class for optimizers defined using COLIN.
- class CollabHybridMetaIterator

  Meta-iterator for hybrid iteration using multiple collaborating optimization and nonlinear least squares methods.
- class GetLongOpt

  GetLongOpt is a general command line utility from S. Manoharan (Advanced Computer Research Institute, Lyon, France).
- class CommandLineHandler

  Utility class for managing command line inputs to DAKOTA.
- class CommandShell

  Utility class which defines convenience operators for spawning processes with system calls.
- class ConcurrentMetaIterator

  Meta-iterator for multi-start iteration or pareto set optimization.
- class CONMINTraits

  A version of TraitsBase specialized for CONMIN optimizers.
- class CONMINOptimizer

  Wrapper class for the CONMIN optimization library.
- class FileReadException

  base class for Dakota file read exceptions (to allow catching both tabular and general file truncation issues)
- class TabularDataTruncated

  exception thrown when data read truncated
- class ResultsFileError

  exception throw for other results file read error
- class FunctionEvalFailure

  exception class for function evaluation failures
- struct BaseConstructor

  Dummy struct for overloading letter-envelope constructors.
- struct NoDBBaseConstructor

  Dummy struct for overloading constructors used in on-the-fly instantiations without ProblemDescDB support.
- struct LightWtBaseConstructor

  Dummy struct for overloading constructors used in on-the-fly Model instantiations.
- struct RealScale

  Data structure for storing real-valued dimension scale.
- struct IntegerScale

  Data structure for storing int-valued dimension scale.
- struct StringScale

  Data structure for storing string-valued dimension scale.
- struct ResultAttribute

  Data structure for a single Real, String, or int valued attribute.
- class ActiveSet

  Container class for active set tracking information. Contains the active set request vector and the derivative variables vector.
- class Analyzer

  Base class for NonD, DACE, and ParamStudy branches of the iterator hierarchy.
- class Approximation

  Base class for the approximation class hierarchy.
- class Constraints

  Base class for the variable constraints class hierarchy.

- class Environment

  Base class for the environment class hierarchy.
- class Graphics

  The Graphics class provides a single interface to 2D (motif) and 3D (PLPLOT) graphics; there is only one instance of this OutputManager::dakotaGraphics.
- class Interface

  Base class for the interface class hierarchy.
- class Iterator

  Base class for the iterator class hierarchy.
- class LeastSq

  Base class for the nonlinear least squares branch of the iterator hierarchy.
- class Minimizer

  Base class for the optimizer and least squares branches of the iterator hierarchy.
- class Model

  Base class for the model class hierarchy.
- class NonD

  Base class for all nondetermistic iterators (the DAKOTA/UQ branch).
- class Optimizer

  Base class for the optimizer branch of the iterator hierarchy.
- class PStudyDACE

  Base class for managing common aspects of parameter studies and design of experiments methods.
- class Response

  Container class for response functions and their derivatives. Response provides the enveloper base class.
- class SurrogatesBaseApprox

  Derived Approximation class for new Surrogates modules.
- class SurrogatesGPApprox

  Derived approximation class for Surrogates approximation classes.
- class SurrogatesPolyApprox

  Derived approximation class for Surrogates Polynomial approximation classes.
- class TPLDataTransfer
- class TraitsBase

  Base class for traits.
- class GeneralReader

  Utility used in derived read_core to read in generic format.
- class TabularReader

  Utility used in derived read_core to read values in tabular format.
- class GeneralWriter

  Utility used in derived write_core to write in generic format.
- class ApreproWriter

  Utility used in derived write_core to write in aprepro format.
- class TabularWriter

  Utility used in derived write_core to write values in tabular format.
- class LabelsWriter

  Utility used in derived write_core to write labels in tabular format.
- class Variables

  Base class for the variables class hierarchy.
- class Verification

  Base class for managing common aspects of verification studies.
- class DataEnvironmentRep

  Body class for environment specification data.
- class DataEnvironment

Handle class for environment specification data.

- class DataFitSurrBasedLocalTraits

  Class for provably-convergent local surrogate-based optimization and nonlinear least squares.
- class DataFitSurrModel

  Derived model class within the surrogate model branch for managing data fit surrogates (global and local)
- class DataInterface

  Handle class for interface specification data.
- class DataMethodRep

  Body class for method specification data.
- class DataMethod

  Handle class for method specification data.
- class DataModelRep

  Body class for model specification data.
- class DataModel

  Handle class for model specification data.
- class DataResponsesRep

  Body class for responses specification data.
- class DataResponses

  Handle class for responses specification data.
- class DataTransformModel

  Data transformation specialization of RecastModel.
- class DataVariablesRep

  Body class for variables specification data.
- class DataVariables

  Handle class for variables specification data.
- class DDACEDesignCompExp

  Wrapper class for the DDACE design of experiments library.
- class DirectApplicInterface

  Derived application interface class which spawns simulation codes and testers using direct procedure calls.
- class DiscrepancyCorrection

  Base class for discrepancy corrections.
- class DLSolverTraits

  A version of TraitsBase specialized for DLSolver.
- class DOTTraits

  Wrapper class for the DOT optimization library.
- class EffGlobalTraits

  Implementation of Efficient Global Optimization/Least Squares algorithms.
- class EffGlobalMinimizer
- class EmbedHybridMetaIterator

  Meta-iterator for closely-coupled hybrid iteration, typically involving the embedding of local search methods within global search methods.
- class EnsembleSurrModel

  Derived model class within the surrogate model branch for managing subordinate models of varying fidelity.
- class ExecutableEnvironment

  Environment corresponding to execution as a stand-alone application.
- class ExperimentData

  Interpolation method for interpolating between experimental and model data. I need to work on inputs/outputs to this method. For now, this assumes interpolation of functional data.
- class ExperimentResponse

  Container class for response functions and their derivatives. ExperimentResponse provides the body class.
- class ForkApplicInterface

Derived application interface class which spawns simulation codes using fork/execvp/waitpid.

- class FSUDesignCompExp

  Wrapper class for the FSUDace QMC/CVT library.

- class GaussProcApproximation

  Derived approximation class for Gaussian Process implementation.

- class GridApplicInterface

  Derived application interface class which spawns simulation codes using grid services such as Condor or Globus.

- class HDF5IOHelper
- class HierarchSurrBasedLocalTraits

  Class for multilevel-multifidelity optimization algorithm.

- class HierarchSurrModel

  Derived model class within the surrogate model branch for managing hierarchical surrogates (models of varying fidelity).

- class IteratorScheduler

  This class encapsulates scheduling operations for concurrent sub-iteration within an outer level context (e.g., meta-iteration, nested models).

- class JEGAOptimizer

  A version of Dakota::Optimizer for instantiation of John Eddy's Genetic Algorithms (JEGA).

- class JEGATraits

  A version of TraitsBase specialized for John Eddy's Genetic Algorithms (JEGA).

- class LibraryEnvironment

  Environment corresponding to execution as an embedded library.

- class MatlabInterface
- class MetaIterator

  Base class for meta-iterators.

- class MinimizerAdapterModel

  Derived model class which wraps call-back functions for solving minimization sub-problems.

- class MixedVarConstraints

  Derived class within the Constraints hierarchy which separates continuous and discrete variables (no domain type array merging).

- class MixedVariables

  Derived class within the Variables hierarchy which separates continuous and discrete variables (no domain type array merging).

- class MPIManager

  Class MPIManager to manage Dakota's MPI world, which may be a subset of MPI_COMM_WORLD.

- class MPIPackBuffer

  Class for packing MPI message buffers.

- class MPIUnpackBuffer

  Class for unpacking MPI message buffers.

- class NCSUTraits

  A version of TraitsBase specialized for NCSU optimizers.

- class NCSUOptimizer

  Wrapper class for the NCSU DIRECT optimization library.

- class NestedModel

  Derived model class which performs a complete sub-iterator execution within every evaluation of the model.

- struct Var_rcheck

  structure for verifying bounds and initial point for real-valued vars

- struct Var_icheck

  structure for verifying bounds and initial point for string-valued vars

- struct VLreal

  structure for validating real uncertain variable labels, bounds, values

- struct VLint

structure for validating integer uncertain variable labels, bounds, values
- struct VLstr

  structure for validating string uncertain variable labels, bounds, values
- class NIDRProblemDescDB

  The derived input file database utilizing the new IDR parser.
- struct NL2Res

  Auxiliary information passed to calcr and calcj via ur.
- class NL2SOLLeastSqTraits

  A version of TraitsBase specialized for NL2SOL nonlinear least squares library.
- class NL2SOLLeastSq

  Wrapper class for the NL2SOL nonlinear least squares library.
- class NLPQLPTraits

  Wrapper class for the NLPQLP optimization library, Version 2.0.
- class NLSSOLLeastSqTraits

  A version of TraitsBase specialized for NLSSOL nonlinear least squares library.
- class NLSSOLLeastSq

  Wrapper class for the NLSSOL nonlinear least squares library.
- class NomadTraits

  Wrapper class for NOMAD Optimizer.
- class NonDACVSampling

  Perform Approximate Control Variate Monte Carlo sampling for UQ.
- class NonDAdaptImpSampling

  Class for the Adaptive Importance Sampling methods within DAKOTA.
- class NonDAdaptiveSampling

  Class for testing various Adaptively sampling methods using geometric, statisctical, and topological information of the surrogate.
- class NonDBayesCalibration

  Base class for Bayesian inference: generates posterior distribution on model parameters given experimental data.
- class NonDC3FunctionTrain

  Nonintrusive uncertainty quantification with the C3 library ...
- class NonDCalibration
- class NonDControlVariateSampling

  Performs Multifidelity Monte Carlo sampling for UQ.
- class NonDCubature

  Derived nondeterministic class that generates N-dimensional numerical cubature points for evaluation of expectation integrals.
- class NonDDREAMBayesCalibration

  Bayesian inference using the DREAM approach.
- class NonDEnsembleSampling

  Base class for Monte Carlo sampling across Model ensembles.
- class NonDExpansion

  Base class for polynomial chaos expansions (PCE), stochastic collocation (SC) and functional tensor train (FT)
- class NonDGlobalEvidence

  Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.
- class NonDGlobalInterval

  Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.
- class NonDGlobalReliability

  Class for global reliability methods within DAKOTA/UQ.
- class NonDGlobalSingleInterval

  Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

- class NonDGPImpSampling

    Class for the Gaussian Process-based Importance Sampling method.
- class NonDGPMSABayesCalibration

    Generates posterior distribution on model parameters given experiment data.
- class NonDHierarchSampling

    Performs Hierarch Monte Carlo sampling for uncertainty quantification.
- class NonDIntegration

    Derived nondeterministic class that generates N-dimensional numerical integration points for evaluation of expectation integrals.
- class NonDInterval

    Base class for interval-based methods within DAKOTA/UQ.
- class NonDLHSEvidence

    Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.
- class NonDLHSInterval

    Class for the LHS-based interval methods within DAKOTA/UQ.
- class NonDLHSSampling

    Performs LHS and Monte Carlo sampling for uncertainty quantification.
- class NonDLHSSingleInterval

    Class for pure interval propagation using LHS.
- class NonDLocalEvidence

    Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.
- class NonDLocalInterval

    Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.
- class NonDLocalReliability

    Class for the reliability methods within DAKOTA/UQ.
- class NonDLocalSingleInterval

    Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.
- class NonDMultifidelitySampling

    Perform Approximate Control Variate Monte Carlo sampling for UQ.
- class NonDMultilevControlVarSampling

    Performs multilevel-multifidelity Monte Carlo sampling for uncertainty quantification.
- class NonDMultilevelFunctionTrain

    Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.
- class NonDMultilevelPolynomialChaos

    Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.
- class NonDMultilevelSampling

    Performs Multilevel Monte Carlo sampling for uncertainty quantification.
- class NonDMultilevelStochCollocation

    Nonintrusive stochastic collocation approaches to uncertainty quantification.
- class NonDMUQBayesCalibration

    Dakota interface to MUQ (MIT Uncertainty Quantification) library.
- class NonDNonHierarchSampling

    Perform Approximate Control Variate Monte Carlo sampling for UQ.
- class NonDPOFDarts

    Base class for POF Dart methods within DAKOTA/UQ.
- class NonDPolynomialChaos

    Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.
- class NonDQuadrature

Derived nondeterministic class that generates N-dimensional numerical quadrature points for evaluation of expectation integrals over uncorrelated standard normals/uniforms/exponentials/betas/gammas.

- class DerivInformedPropCovTK

  Dakota transition kernel that updates proposal covariance based on derivatives (for random walk case)
- class DerivInformedPropCovLogitTK

  Dakota transition kernel that updates proposal covariance based on derivatives (for logit random walk case)
- class NonDQUESOBayesCalibration

  Bayesian inference using the QUESO library from UT Austin.
- class NonDReliability

  Base class for the reliability methods within DAKOTA/UQ.
- class NonDRKDDarts

  Base class for the Recursive k-d Dart methods within DAKOTA/UQ.
- class NonDSampling

  Base class for common code between NonDLHSSampling, NonDAdaptImpSampling, and other specializations.
- class NonDSparseGrid

  Derived nondeterministic class that generates N-dimensional Smolyak sparse grids for numerical evaluation of expectation integrals over independent standard random variables.
- class NonDStochCollocation

  Nonintrusive stochastic collocation approaches to uncertainty quantification.
- class NonDSurrogateExpansion

  Generic uncertainty quantification with Model-based stochastic expansions.
- class NonDWASABIBayesCalibration

  WASABI - Weighted Adaptive Surrogate Approximations for Bayesian Inference.
- class NonHierarchSurrModel

  Derived model class within the surrogate model branch for managing unordered surrogate models of varying fidelity.
- class NonlinearCGTraits

  A version of TraitsBase specialized for NonlinearCG optimizers.
- class NonlinearCGOptimizer
- class NOWPACBlackBoxEvaluator

  Derived class for plugging Dakota evaluations into NOWPAC solver.
- class NOWPACTraits

  A version of TraitsBase specialized for NOWPAC optimizers.
- class NOWPACOptimizer

  Wrapper class for the (S)NOWPAC optimization algorithms from Florian Augustin (MIT)
- class NPSOLTraits

  Wrapper class for the NPSOL optimization library.
- class OptDartsTraits

  A version of TraitsBase specialized for OptDarts.
- class OptDartsOptimizer

  Wrapper class for OptDarts Optimizer.
- class OutputWriter
- class ConsoleRedirector
- class RestartWriter
- class OutputManager

  Class to manage redirection of stdout/stderr, keep track of current redir state, and manage rank 0 output. Also manage tabular data output for post-processing with Matlab, Tecplot, etc. and delegate to Graphics for X Windows Graphics.
- class ParallelLevel

  Container class for the data associated with a single level of communicator partitioning.
- class ParallelConfiguration

  Container class for a set of ParallelLevel list iterators that collectively identify a particular multilevel parallel configuration.
- class ParallelLibrary

Class for partitioning multiple levels of parallelism and managing message passing within these levels.

- class ParamResponsePair

  Container class for a variables object, a response object, and an evaluation id.
- class ParamStudy

  Class for vector, list, centered, and multidimensional parameter studies.
- class PebbldBranching

  Main Branching class for the PEBBL-based Minimizer.
- class PebbldBranchSub

  Sub Branch class for the PEBBL-based Minimizer.
- class PebbldTraits

  Wrapper class for experimental PebbldMinimizer.
- class PecosApproximation

  Derived approximation class for global basis polynomials.
- class ProbabilityTransformModel

  Probability transformation specialization of RecastModel.
- class ProblemDescDB

  The database containing information parsed from the DAKOTA input file.
- class ProcessApplicInterface

  Derived application interface class that spawns a simulation code using a separate process and communicates with it through files.
- class ProcessHandleApplicInterface

  Derived application interface class that spawns a simulation code using a separate process, receives a process identifier, and communicates with the spawned process through files.
- class ProgramOptions

  ProgramOptions stores options whether from the CLH or from library user; initially valid only on worldRank = 0, but then broadcast in ParallelLibrary::push_output_tag()
- struct partial_prp_hash

  wrapper to delegate to the ParamResponsePair hash_value function
- struct partial_prp_equality

  predicate for comparing ONLY the interfaceId and Vars attributes of PRPair
- class PSUADEDesignCompExp

  Wrapper class for the PSUADE library.
- class Pybind11Interface
- class PythonInterface
- class QMEApproximation

  Derived approximation class for QMEA Quadratic Multipoint Exponential Approximation (a multipoint approximation).
- class QuesoJointPdf

  Dakota specialization of QUESO generic joint PDF.
- class QuesoVectorRV

  Dakota specialization of QUESO vector-valued random variable.
- class TKFactoryDIPC

  Custom RW TKfactory: passes Dakota QUESO instance pointer to the TK at build.
- class TKFactoryDIPCLogit

  Custom Logit RW TKfactory: passed Dakota QUESO instance pointer to the TK at build.
- class RandomFieldModel

  Random field model, capable of generating and then forward propagating.
- class RecastModel

  Derived model class which provides a thin wrapper around a sub-model in order to recast the form of its inputs and/or outputs.
- class ReducedBasis
- class RelaxedVarConstraints

  Derived class within the Constraints hierarchy which employs relaxation of discrete variables.

- class RelaxedVariables

  Derived class within the Variables hierarchy which employs the relaxation of discrete variables.
- class ResultsDBAny
- class ResultsDBBase
- class AddAttributeVisitor

  Objects of this class are called by boost::appy_visitor to add attributes to HDF5 objects.
- class AttachScaleVisitor

  Objects of this class are called by boost::appy_visitor to add dimension scales (RealScale or StringScale) to HDF5 datasets.
- class ResultsDBHDF5

  Manage interactions between ResultsManager and the low-level HDFIOHelper class.
- class ResultsNames

  List of valid names for iterator results.
- class ResultsManager

  Results manager for iterator final data.
- class ResultsEntry

  Class to manage in-core vs. file database lookups.
- class RichExtrapVerification

  Class for Richardson extrapolation for code and solution verification.
- class ROLOptimizer
- class ROLTraits
- class DakotaROLObjective
- class DakotaROLObjectiveGrad
- class DakotaROLObjectiveHess
- class DakotaROLIneqConstraints
- class DakotaROLIneqConstraintsGrad
- class DakotaROLIneqConstraintsHess
- class DakotaROLEqConstraints
- class DakotaROLEqConstraintsGrad
- class DakotaROLEqConstraintsHess
- class PrefixingLineFilter
- class ScalingModel

  Scaling specialization of RecastModel.
- class ScalingOptions

  Simple container for user-provided scaling data, possibly expanded by replicates through the models.
- class ScilabInterface
- class SensAnalysisGlobal

  Class for a utility class containing correlation calculations and variance-based decomposition.
- class SeqHybridMetaIterator

  Method for sequential hybrid iteration using multiple optimization and nonlinear least squares methods on multiple models of varying fidelity.
- class SharedApproxData

  Base class for the shared approximation data class hierarchy.
- class SharedC3ApproxData

  Derived approximation class for global basis polynomials.
- class SharedPecosApproxData

  Derived approximation class for global basis polynomials.
- class SharedResponseDataRep

  The representation of a SharedResponseData instance. This representation, or body, may be shared by multiple SharedResponseData handle instances.
- class SharedResponseData

  Container class encapsulating variables data that can be shared among a set of Response instances.

- class SharedSurfpackApproxData

  Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.
- class SharedVariablesDataRep

  The representation of a SharedVariablesData instance. This representation, or body, may be shared by multiple SharedVariablesData handle instances.
- class SharedVariablesData

  Container class encapsulating variables data that can be shared among a set of Variables instances.
- class SimulationModel

  Derived model class which utilizes a simulation-based application interface to map variables into responses.
- class SimulationResponse

  Container class for response functions and their derivatives. SimulationResponse provides the body class.
- class SNLLBase

  Base class for OPT++ optimization and least squares methods.
- class SNLLLeastSqTraits

  A version of TraitsBase specialized for SNLLLeastSq.
- class SNLLLeastSq

  Wrapper class for the OPT++ optimization library.
- class SNLLTraits

  A version of TraitsBase specialized for SNLL optimizers.
- class SNLLOptimizer

  Wrapper class for the OPT++ optimization library.
- class SOLBase

  Base class for Stanford SOL software.
- class SpawnApplicInterface

  Derived application interface class which spawns simulation codes using spawnvp.
- class SubspaceModel

  Subspace model for input (variable space) reduction.
- class SurfpackApproximation

  Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.
- class SurrBasedGlobalTraits

  The global surrogate-based minimizer which sequentially minimizes and updates a global surrogate model without trust region controls.
- class SurrBasedGlobalMinimizer
- class SurrBasedLocalMinimizer

  Class for provably-convergent local surrogate-based optimization and nonlinear least squares.
- class SurrBasedMinimizer

  Base class for local/global surrogate-based optimization/least squares.
- class SurrogateModel

  Base class for surrogate models (DataFitSurrModel and HierarchSurrModel).
- class SysCallApplicInterface

  Derived application interface class which spawns simulation codes using system calls.
- class TANA3Approximation

  Derived approximation class for TANA-3 two-point exponential approximation (a multipoint approximation).
- class TaylorApproximation

  Derived approximation class for first- or second-order Taylor series (a local approximation).
- class TestDriverInterface
- class TrackerHTTP

  TrackerHTTP: a usage tracking module that uses HTTP/HTTPS via the curl library.
- class UsageTracker

  Lightweight class to manage conditionally active Curl-based HTTP tracker via PIMPL.
- class VPSApproximation

Derived approximation class for VPS implementation.

- class WeightingModel

  Weighting specialization of RecastModel.

- struct MatchesWC

  Predicate that returns true when the passed path matches the wild_card with which it was configured. Currently supports ∗ and ?.

- class WorkdirHelper

Typedefs

- typedef boost::tuple
  < std::string, std::string,
  size_t, std::string > ResultsKeyType

  Data type for results key (instance name / id, unique run, label), where data_key is a valid colon-delimited string from ResultsNames tuple<method_name, method_id, execution_number, data_key>

- typedef std::string MetaDataKeyType

  Data type for metadata key.

- typedef std::vector< std::string > MetaDataValueType

  Data type for metadata value.

- typedef std::map
  < MetaDataKeyType,
  MetaDataValueType > MetaDataType

  A single MetaData entry is map<string, vector<string> > Example: pair("Column labels", ["Mean", "Std Dev", "Skewness", "Kurtosis"])

- typedef boost::tuple
  < std::string, std::string,
  size_t > StrStrSizet

  Iterator unique ID: <method_name, method_id, exec_num>

- typedef std::multimap< int,
  boost::variant< StringScale,
  RealScale, IntegerScale > > DimScaleMap

  Datatype to communicate scales (stored in boost::variant) and their associated dimension (the int) to the Results-Manager instance.

- typedef std::vector
  < boost::variant
  < ResultAttribute< int >
  , ResultAttribute< String >
  , ResultAttribute< Real > > > AttributeArray

  Datatype to communcate metadata (attributes) to the ResultsManager instance.

- typedef boost::bimap< unsigned
  short, std::string > UShortStrBimap

  bimaps to convert from enums <–> strings

- using **RespMetadataT** = double
- typedef void(∗ **dl_core_run_t**)(void ∗, Optimizer1 ∗, char ∗)
- typedef void(∗ **dl_destructor_t**)(void ∗∗)
- typedef
  Teuchos::SerialDenseSolver
  < int, Real > **RealSolver**
- typedef
  Teuchos::SerialSpdDenseSolver
  < int, Real > **RealSpdSolver**
- typedef int(∗ start_grid_computing_t)(char ∗analysis_driver_script, char ∗params_file, char ∗results_file)

  definition of start grid computing type (function pointer)

- typedef int(∗ perform_analysis_t)(char ∗iteration_num) *definition of perform analysis type (function pointer)*

- typedef int ∗(∗ get_jobs_completed_t)()

  definition of get completed jobs type (function pointer)

- typedef int(∗ stop_grid_computing_t)()

  definition of stop grid computing type (function pointer)

- typedef int **MPI_Comm**
- typedef void ∗ **MPI_Request**
- typedef unsigned char **u_char**
- typedef unsigned short **u_short**
- typedef unsigned int **u_int**
- typedef unsigned long **u_long**
- typedef long long **long_long**
- typedef unsigned long **UL**
- typedef void(∗ **Calcrj**)(int ∗n, int ∗p, Real ∗x, int ∗nf, Real ∗r, int ∗ui, void ∗ur, Vf vf)
- typedef void(∗ **Vf**)()
- typedef void(∗ **DbCallbackFunctionPtr**)(Dakota::ProblemDescDB ∗db, void ∗data_ptr)
- typedef boost::tuple
  < bfs::path, bfs::path,
  bfs::path > PathTriple

  Triplet of filesystem paths: e.g., params, results, workdir.

- typedef
  bmi::multi_index_container
  < Dakota::ParamResponsePair,
  bmi::indexed_by
  < bmi::ordered_non_unique
  < bmi::tag< ordered >
  , bmi::const_mem_fun
  < Dakota::ParamResponsePair,
  const IntStringPair
  &,&Dakota::ParamResponsePair::eval_interface_ids >
  >, bmi::hashed_non_unique
  < bmi::tag< hashed >
  , bmi::identity
  < Dakota::ParamResponsePair >
  , partial_prp_hash,
  partial_prp_equality > > > PRPMultiIndexCache

  Boost Multi-Index Container for globally caching ParamResponsePairs.

- typedef PRPMultiIndexCache **PRPCache**
- typedef
  PRPCache::index_iterator
  < ordered >::type **PRPCacheOIter**
- typedef
  PRPCache::index_const_iterator
  < ordered >::type **PRPCacheOCIter**
- typedef
  PRPCache::index_iterator
  < hashed >::type **PRPCacheHIter**
- typedef
  PRPCache::index_const_iterator
  < hashed >::type **PRPCacheHCIter**
- typedef PRPCacheOIter PRPCacheIter

  default cache iterator <0>

- typedef PRPCacheOCIter PRPCacheCIter

  `default cache const iterator <0>`

  default cache const reverse iterator <0>

- typedef boost::reverse_iterator < PRPCacheCIter > **PRPCacheCRevIter**
- typedef bmi::multi_index_container < Dakota::ParamResponsePair, bmi::indexed_by < bmi::ordered_unique < bmi::tag< ordered > , bmi::const_mem_fun < Dakota::ParamResponsePair, int,&Dakota::ParamResponsePair::eval_id > >, bmi::hashed_non_unique < bmi::tag< hashed > , bmi::identity < Dakota::ParamResponsePair > , partial_prp_hash, partial_prp_equality > > > PRPMultiIndexQueue

  Boost Multi-Index Container for locally queueing ParamResponsePairs.
- typedef PRPMultiIndexQueue **PRPQueue**
- typedef PRPQueue::index_iterator < ordered >::type **PRPQueueOIter**
- typedef PRPQueue::index_const_iterator < ordered >::type **PRPQueueOCIter**
- typedef PRPQueue::index_iterator < hashed >::type **PRPQueueHIter**
- typedef PRPQueue::index_const_iterator < hashed >::type **PRPQueueHCIter**
- typedef PRPQueueOIter **PRPQueueIter**
- typedef PRPQueueOCIter **PRPQueueCIter**
- typedef std::pair< boost::any, MetaDataType > ResultsValueType

  Core data storage type: boost::any, with optional metadata (see other types in results_types.hpp)
- typedef boost::function< bool(const bfs::path &src_path, const bfs::path &dest_path, bool overwrite)> file_op_function

  define a function type that operates from src to dest, with option to overwrite
- typedef boost::filter_iterator < MatchesWC, bfs::directory_iterator > glob_iterator

  a glob_iterator filters a directory_iterator based on a wildcard predicate

Enumerations

- enum { **COBYLA**, **DIRECT**, **EA**, **MS**, **PS**, **SW**, **BETA** }
- enum { **VARS_ERROR** = -10, **RESP_ERROR** = -9, **APPROX_ERROR** = -8, **METHOD_ERROR** = -7, **MODEL_ERROR** = -6, **IO_ERROR** = -5, **INTERFACE_ERROR** = -4, **CONSTRUCT_ERROR** = -3, **PARSE_ERROR** = -2, **OTHER_ERROR** = -1 }

enum for Dakota abort reasons; using negative numbers to distinguish Dakota exit states from signals / uncaught signals. These need to be in range [-63, -1], so exit code (256+enum) is in [193, 255]. See RATIONALE in dakota_-global_defs.cpp.

- enum { **MODEL_EVAL_STORE_TOP_METHOD** = 0, **MODEL_EVAL_STORE_NONE**, **MODEL_EVAL_ST-ORE_ALL**, **MODEL_EVAL_STORE_ALL_METHODS** }

  enum for selecting the models that store evaluations

- enum { **INTERF_EVAL_STORE_SIMULATION** = 0, **INTERF_EVAL_STORE_NONE**, **INTERF_EVAL_STO-RE_ALL** }

  enum for selecting the interfaces that store evaluations

- enum { **ABORT_EXITS**, **ABORT_THROWS** }

  enum for dakota abort behaviors

- enum { **CV_ID_DEFAULT** = 0, **MINIMUM_METRIC**, **RELATIVE_TOLERANCE**, **DECREASE_TOLERANCE** }

  enum for active subspace cross validation identification

- enum {
  TABULAR_NONE = 0, **TABULAR_HEADER** = 1, **TABULAR_EVAL_ID** = 2, **TABULAR_IFACE_ID** = 4, **TABULAR_EXPER_ANNOT** = TABULAR_HEADER | TABULAR_EVAL_ID, **TABULAR_ANNOTATED** = T-ABULAR_HEADER | TABULAR_EVAL_ID | TABULAR_IFACE_ID }

  options for tabular columns

- enum { **RESULTS_OUTPUT_TEXT** = 1, **RESULTS_OUTPUT_HDF5** = 2 }

  Results output format.

- enum { **FLEXIBLE_RESULTS**, **LABELED_RESULTS** }

  options for results file format

- enum {
  NO_MODEL_FORMAT =0, **TEXT_ARCHIVE** =1, **BINARY_ARCHIVE** =2, **ALGEBRAIC_FILE** =4, **ALGEBRAIC_CONSOLE** =8 }

  define special values for surrogateExportFormats

- enum ScaleScope { **SHARED**, **UNSHARED** }

  Enum to specify whether a scale shared among responses.

- enum ResultsOutputType { **REAL**, **INTEGER**, **UINTEGER**, **STRING** }

  enum for setting type on allocted matrix for Results Output

- enum **CONSTRAINT_TYPE** { **LINEAR**, **NONLINEAR** }
- enum **CONSTRAINT_EQUALITY_TYPE** { **EQUALITY**, **INEQUALITY** }
- enum **LINEAR_INEQUALITY_FORMAT** { **NONE**, **TWO_SIDED**, **ONE_SIDED_LOWER**, **ONE_SIDED_UP-PER** }
- enum **NONLINEAR_EQUALITY_FORMAT** { **NONE**, **TRUE_EQUALITY**, **TWO_INEQUALITY** }
- enum **NONLINEAR_INEQUALITY_FORMAT** { **NONE**, **ONE_SIDED_UPPER**, **ONE_SIDED_LOWER**, **TW-O_SIDED** }
- enum {
  DEFAULT_INTERFACE =0, **APPROX_INTERFACE**, **FORK_INTERFACE** =PROCESS_INTERFACE_BIT, **SYSTEM_INTERFACE**,
  GRID_INTERFACE, **TEST_INTERFACE** =DIRECT_INTERFACE_BIT, **PLUGIN_INTERFACE**, **MATLAB_I-NTERFACE**,
  LEGACY_PYTHON_INTERFACE, **PYTHON_INTERFACE**, **SCILAB_INTERFACE** }

  special values for interface type

- enum { **SYNCHRONOUS_INTERFACE**, **ASYNCHRONOUS_INTERFACE** }

  interface synchronization types

- enum { **OBJECTIVE**, **INEQUALITY_CONSTRAINT**, **EQUALITY_CONSTRAINT** }

  define algebraic function types

- enum {
DEFAULT_METHOD =0, **HYBRID** =(META_BIT | PARALLEL_BIT), **PARETO_SET**, **MULTI_START**,
RICHARDSON_EXTRAP =(ANALYZER_BIT | VERIF_BIT), **CENTERED_PARAMETER_STUDY** =(ANALYZER_BIT | PSTUDYDACE_BIT), **LIST_PARAMETER_STUDY**, **MULTIDIM_PARAMETER_STUDY**,
VECTOR_PARAMETER_STUDY, **DACE**, **FSU_CVT**, **FSU_HALTON**,
FSU_HAMMERSLEY, **PSUADE_MOAT**, **LOCAL_RELIABILITY** =(ANALYZER_BIT | NOND_BIT), **GLOBAL_RELIABILITY**,
SURROGATE_BASED_UQ, **POLYNOMIAL_CHAOS**, **MULTILEVEL_POLYNOMIAL_CHAOS**, **MULTIFIDELITY_POLYNOMIAL_CHAOS**,
STOCH_COLLOCATION, **MULTIFIDELITY_STOCH_COLLOCATION**, **C3_FUNCTION_TRAIN**, **MULTILEVEL_FUNCTION_TRAIN**,
MULTIFIDELITY_FUNCTION_TRAIN, **CUBATURE_INTEGRATION**, **SPARSE_GRID_INTEGRATION**, **QUADRATURE_INTEGRATION**,
BAYES_CALIBRATION, **GPAIS**, **POF_DARTS**, **RKD_DARTS**,
IMPORTANCE_SAMPLING, **ADAPTIVE_SAMPLING**, **MULTILEVEL_SAMPLING**, **MULTIFIDELITY_SAMPLING**,
MULTILEVEL_MULTIFIDELITY_SAMPLING, **APPROXIMATE_CONTROL_VARIATE**, **LIST_SAMPLING**,
RANDOM_SAMPLING,
LOCAL_INTERVAL_EST, **LOCAL_EVIDENCE**, **GLOBAL_INTERVAL_EST**, **GLOBAL_EVIDENCE**,
SURROGATE_BASED_LOCAL =(MINIMIZER_BIT | SURRBASED_BIT), **DATA_FIT_SURROGATE_BASED_LOCAL**, **HIERARCH_SURROGATE_BASED_LOCAL**, **SURROGATE_BASED_GLOBAL**,
EFFICIENT_GLOBAL, **NL2SOL** =(MINIMIZER_BIT | LEASTSQ_BIT), **NLSSOL_SQP**, **OPTPP_G_NEWTON**,
ASYNCH_PATTERN_SEARCH =(MINIMIZER_BIT | OPTIMIZER_BIT), **OPTPP_PDS**, **COLINY_BETA**, **COLINY_COBYLA**,
COLINY_DIRECT, **COLINY_MULTI_START**, **COLINY_EA**, **COLINY_PATTERN_SEARCH**,
COLINY_SOLIS_WETS, **MOGA**, **SOGA**, **NCSU_DIRECT**,
MESH_ADAPTIVE_SEARCH, **MIT_NOWPAC**, **MIT_SNOWPAC**, **GENIE_OPT_DARTS**,
GENIE_DIRECT, **DEMO_TPL**, **NONLINEAR_CG**, **OPTPP_CG**,
OPTPP_Q_NEWTON, **OPTPP_FD_NEWTON**, **OPTPP_NEWTON**, **NPSOL_SQP**,
NLPQL_SQP, **DOT_BFGS**, **DOT_FRCG**, **DOT_MMFD**,
DOT_SLP, **DOT_SQP**, **CONMIN_FRCG**, **CONMIN_MFD**,
ROL, **DL_SOLVER**, **BRANCH_AND_BOUND** =(MINIMIZER_BIT | OPTIMIZER_BIT | LEASTSQ_BIT) }
- enum {
SUBMETHOD_DEFAULT =0, **SUBMETHOD_NONE**, SUBMETHOD_COLLABORATIVE, **SUBMETHOD_EMBEDDED**,
SUBMETHOD_SEQUENTIAL, **SUBMETHOD_LHS**, **SUBMETHOD_RANDOM**, **SUBMETHOD_BOX_BEHNKEN**,
SUBMETHOD_CENTRAL_COMPOSITE, **SUBMETHOD_GRID**, **SUBMETHOD_OA_LHS**, **SUBMETHOD_OAS**,
SUBMETHOD_MFMC, **SUBMETHOD_ACV_IS**, **SUBMETHOD_ACV_MF**, **SUBMETHOD_ACV_KL**,
SUBMETHOD_DREAM, **SUBMETHOD_GPMSA**, **SUBMETHOD_MUQ**, **SUBMETHOD_QUESO**,
SUBMETHOD_WASABI, **SUBMETHOD_CONMIN**, **SUBMETHOD_DOT**, **SUBMETHOD_NLPQL**,
SUBMETHOD_NPSOL, **SUBMETHOD_OPTPP**, **SUBMETHOD_EA**, **SUBMETHOD_DIRECT**,
SUBMETHOD_EGO, **SUBMETHOD_SBLO**, **SUBMETHOD_SBGO**, **SUBMETHOD_AMV_X**,
SUBMETHOD_AMV_U, **SUBMETHOD_AMV_PLUS_X**, **SUBMETHOD_AMV_PLUS_U**, **SUBMETHOD_TANA_X**,
SUBMETHOD_TANA_U, **SUBMETHOD_QMEA_X**, **SUBMETHOD_QMEA_U**, **SUBMETHOD_NO_APPROX**,
SUBMETHOD_EGRA_X, **SUBMETHOD_EGRA_U**, **SUBMETHOD_CONVERGE_ORDER**, **SUBMETHOD_CONVERGE_QOI**,
SUBMETHOD_ESTIMATE_ORDER }

  Sub-methods, including sampling, inference algorithm, opt algorithm types.
- enum {
SILENT_OUTPUT, **QUIET_OUTPUT**, **NORMAL_OUTPUT**, **VERBOSE_OUTPUT**,
DEBUG_OUTPUT }
- enum { **NO_RESULTS** =0, **REFINEMENT_RESULTS**, **INTERMEDIATE_RESULTS**, **FINAL_RESULTS** }
- enum { **DEFAULT_SYNCHRONIZATION** =0, **BLOCKING_SYNCHRONIZATION**, **NONBLOCKING_SYNC-**

HRONIZATION }
- enum {
DEFAULT_SCHEDULING, **MASTER_SCHEDULING**, **PEER_SCHEDULING**, **PEER_DYNAMIC_SCHEDULING**,
PEER_STATIC_SCHEDULING, **DYNAMIC_SCHEDULING**, **STATIC_SCHEDULING** }
- enum { **DEFAULT_CONFIG**, **PUSH_DOWN**, **PUSH_UP** }
- enum {
STD_NORMAL_U, **STD_UNIFORM_U**, **PARTIAL_ASKEY_U**, **ASKEY_U**,
EXTENDED_U }
- enum { **DEFAULT_COVARIANCE**, **NO_COVARIANCE**, **DIAGONAL_COVARIANCE**, **FULL_COVARIANCE** }
- enum { **NO_INT_REFINE** =0, **IS**, **AIS**, **MMAIS** }
- enum { **PROBABILITIES**, **RELIABILITIES**, **GEN_RELIABILITIES** }
- enum { **COMPONENT** =0, **SYSTEM_SERIES**, **SYSTEM_PARALLEL** }
- enum { **CUMULATIVE**, **COMPLEMENTARY** }
- enum { **DEFAULT_LS** =0, **SVD_LS**, **EQ_CON_LS** }
- enum {
DEFAULT_MLMF_CONTROL =0, **ESTIMATOR_VARIANCE**, **RIP_SAMPLING**, **RANK_SAMPLING**,
GREEDY_REFINEMENT }
- enum { **DEFAULT_EMULATION**, **DISTINCT_EMULATION**, **RECURSIVE_EMULATION** }
- enum {
NO_EMULATOR, **PCE_EMULATOR**, **ML_PCE_EMULATOR**, **MF_PCE_EMULATOR**,
SC_EMULATOR, **MF_SC_EMULATOR**, **GP_EMULATOR**, **KRIGING_EMULATOR**,
EXPGP_EMULATOR, **VPS_EMULATOR** }
- enum {
CALIBRATE_NONE = 0, **CALIBRATE_ONE**, **CALIBRATE_PER_EXPER**, **CALIBRATE_PER_RESP**,
CALIBRATE_BOTH }
- enum { **IGNORE_RANKS**, **SET_RANKS**, **GET_RANKS**, **SET_GET_RANKS** }
- enum {
DESIGN, **UNCERTAIN**, **UNCERTAIN_UNIFORM**, **ALEATORY_UNCERTAIN**,
ALEATORY_UNCERTAIN_UNIFORM, **EPISTEMIC_UNCERTAIN**, **EPISTEMIC_UNCERTAIN_UNIFORM**,
STATE,
ACTIVE, **ACTIVE_UNIFORM**, **ALL**, **ALL_UNIFORM** }
- enum {
ONE_SIDED_LOWER, **ONE_SIDED_LOWER**, **ONE_SIDED_LOWER**, **ONE_SIDED_UPPER**,
ONE_SIDED_UPPER, **ONE_SIDED_UPPER**, **TWO_SIDED**, **TWO_SIDED**,
TWO_SIDED }
- enum { **NO_FINAL_STATS** =0, **QOI_STATISTICS**, **ESTIMATOR_PERFORMANCE** }
- enum { **QOI_AGGREGATION_MAX**, **QOI_AGGREGATION_SUM** }
- enum { **TARGET_MEAN**, **TARGET_VARIANCE**, **TARGET_SIGMA**, **TARGET_SCALARIZATION** }
- enum { **CONVERGENCE_TOLERANCE_TYPE_RELATIVE**, **CONVERGENCE_TOLERANCE_TYPE_ABSOLUTE** }
- enum { **CONVERGENCE_TOLERANCE_TARGET_VARIANCE_CONSTRAINT**, **CONVERGENCE_TOLERANCE_TARGET_COST_CONSTRAINT** }
- enum { **ONLINE_PILOT**, **OFFLINE_PILOT**, **PILOT_PROJECTION** }
- enum { **REORDERED_FALLBACK**, **NUMERICAL_FALLBACK**, **NUMERICAL_OVERRIDE** }
- enum { **BREITUNG**, **HOHENRACK**, **HONG** }
- enum { **ORIGINAL_PRIMARY**, **SINGLE_OBJECTIVE**, **LAGRANGIAN_OBJECTIVE**, **AUGMENTED_LAGRANGIAN_OBJECTIVE** }
- enum { **NO_CONSTRAINTS**, **LINEARIZED_CONSTRAINTS**, **ORIGINAL_CONSTRAINTS** }
- enum { **NO_RELAX**, **HOMOTOPY**, **COMPOSITE_STEP** }
- enum { **PENALTY_MERIT**, **ADAPTIVE_PENALTY_MERIT**, **LAGRANGIAN_MERIT**, **AUGMENTED_LAGRANGIAN_MERIT** }
- enum { **FILTER**, **TR_RATIO** }
- enum { **DEFAULT_POINTS**, **MINIMUM_POINTS**, **RECOMMENDED_POINTS**, **TOTAL_POINTS** }

    define special values for pointsManagement

- enum {
NO_SURROGATE =0, **UNCORRECTED_SURROGATE**, **AUTO_CORRECTED_SURROGATE**, **BYPASS_-SURROGATE**,
MODEL_DISCREPANCY, **AGGREGATED_MODELS** }

  define special values for SurrogateModel::responseMode
- enum { **NO_CORRECTION** =0, **ADDITIVE_CORRECTION**, **MULTIPLICATIVE_CORRECTION**, **COMBINE-D_CORRECTION** }

  define special values for approxCorrectionType
- enum { **RF_KARHUNEN_LOEVE** =0, **RF_PCA_GP**, **RF_ICA** }

  define types of random field approximations
- enum { **NOCOVAR** =0, **EXP_L2**, **EXP_L1** }

  define types of analytic covariance functions
- enum { **SUBSPACE_NORM_DEFAULT** =0, **SUBSPACE_NORM_MEAN_VALUE**, **SUBSPACE_NORM_M-EAN_GRAD**, **SUBSPACE_NORM_LOCAL_GRAD** }

  define special values for active subspace normalizations
- enum { **ROTATION_METHOD_UNRANKED**, **ROTATION_METHOD_RANKED** }
- enum {
NO_PARALLEL_MODE =0, **SURROGATE_MODEL_MODE**, **TRUTH_MODEL_MODE**, **SUB_MODEL_M-ODE**,
INTERFACE_MODE }

  define special values for componentParallelMode (active model for parallel scheduling)
- enum { **NO_DERIVS** =0, **ALL_DERIVS**, **MIXED_DERIVS** }

  define special values for distParamDerivs
- enum { **FT_LS**, **FT_RLS2** }
- enum {
NO_C3_ADVANCEMENT =0, **START_RANK_ADVANCEMENT**, **START_ORDER_ADVANCEMENT**, **MA-X_RANK_ADVANCEMENT**,
MAX_ORDER_ADVANCEMENT, **MAX_RANK_ORDER_ADVANCEMENT** }
- enum { **BASE_RESPONSE** =0, **SIMULATION_RESPONSE**, **EXPERIMENT_RESPONSE** }

  special values for derived Response type
- enum { **GENERIC_FNS** = 0, **OBJECTIVE_FNS**, **CALIB_TERMS** }

  values for primary response types
- enum { **DEFAULT_DOMAIN** =0, **RELAXED_DOMAIN**, **MIXED_DOMAIN** }
- enum {
DEFAULT_VIEW =0, **ALL_VIEW**, **DESIGN_VIEW**, **UNCERTAIN_VIEW**,
ALEATORY_UNCERTAIN_VIEW, **EPISTEMIC_UNCERTAIN_VIEW**, **STATE_VIEW** }
- enum {
EMPTY_VIEW =0, **RELAXED_ALL**, **MIXED_ALL**, **RELAXED_DESIGN**,
RELAXED_UNCERTAIN, **RELAXED_ALEATORY_UNCERTAIN**, **RELAXED_EPISTEMIC_UNCERTAIN**, **RELAXED_STATE**,
MIXED_DESIGN, **MIXED_UNCERTAIN**, **MIXED_ALEATORY_UNCERTAIN**, **MIXED_EPISTEMIC_UNCE-RTAIN**,
MIXED_STATE }
- enum { **ALL_VARS** =0, **ACTIVE_VARS**, **INACTIVE_VARS** }

  values differentiating subsets of variables for I/O
- enum {
EMPTY_TYPE =0, **CONTINUOUS_DESIGN**, **DISCRETE_DESIGN_RANGE**, **DISCRETE_DESIGN_SET_I-NT**,
DISCRETE_DESIGN_SET_STRING, **DISCRETE_DESIGN_SET_REAL**, **NORMAL_UNCERTAIN**, **LOGN-ORMAL_UNCERTAIN**,
UNIFORM_UNCERTAIN, **LOGUNIFORM_UNCERTAIN**, **TRIANGULAR_UNCERTAIN**, **EXPONENTIAL_U-NCERTAIN**,
BETA_UNCERTAIN, **GAMMA_UNCERTAIN**, **GUMBEL_UNCERTAIN**, **FRECHET_UNCERTAIN**,
WEIBULL_UNCERTAIN, **HISTOGRAM_BIN_UNCERTAIN**, **POISSON_UNCERTAIN**, **BINOMIAL_UNCE-RTAIN**,
NEGATIVE_BINOMIAL_UNCERTAIN, **GEOMETRIC_UNCERTAIN**, **HYPERGEOMETRIC_UNCERTAIN**,

HISTOGRAM_POINT_UNCERTAIN_INT, **HISTOGRAM_POINT_UNCERTAIN_STRING**, **HISTOGRAM_POINT_UNCERTAIN_REAL**, **CONTINUOUS_INTERVAL_UNCERTAIN**, **DISCRETE_INTERVAL_UNCERTAIN**, **DISCRETE_UNCERTAIN_SET_INT**, **DISCRETE_UNCERTAIN_SET_STRING**, **DISCRETE_UNCERTAIN_SET_REAL**, **CONTINUOUS_STATE**, **DISCRETE_STATE_RANGE**, **DISCRETE_STATE_SET_INT**, **DISCRETE_STATE_SET_STRING**, **DISCRETE_STATE_SET_REAL** }

- enum {
  TOTAL_CDV =0, **TOTAL_DDIV**, **TOTAL_DDSV**, **TOTAL_DDRV**,
  TOTAL_CAUV, **TOTAL_DAUIV**, **TOTAL_DAUSV**, **TOTAL_DAURV**,
  TOTAL_CEUV, **TOTAL_DEUIV**, **TOTAL_DEUSV**, **TOTAL_DEURV**,
  TOTAL_CSV, **TOTAL_DSIV**, **TOTAL_DSSV**, **TOTAL_DSRV**,
  NUM_VC_TOTALS }
- enum var_t {
  VAR_x1, **VAR_x2**, **VAR_x3**, **VAR_b**,
  VAR_h, **VAR_P**, **VAR_M**, **VAR_Y**,
  VAR_w, **VAR_t**, **VAR_R**, **VAR_E**,
  VAR_X, **VAR_area_type**, **VAR_Fs**, **VAR_P1**,
  VAR_P2, **VAR_P3**, **VAR_B**, **VAR_D**,
  VAR_H, **VAR_F0**, **VAR_d**, **VAR_MForm**,
  VAR_x, **VAR_xi**, **VAR_Af**, **VAR_Ac**,
  VAR_y, **VAR_theta**, **VAR_theta1**, **VAR_theta2**,
  VAR_delta, **VAR_gamma** }

  enumeration of possible variable types (to index to names)
- enum driver_t {
  NO_DRIVER =0, **CANTILEVER_BEAM**, **MOD_CANTILEVER_BEAM**, **CANTILEVER_BEAM_ML**,
  CYLINDER_HEAD, **EXTENDED_ROSENBROCK**, **GENERALIZED_ROSENBROCK**, **LF_ROSENBROCK**,
  EXTRA_LF_ROSENBROCK, **MF_ROSENBROCK**, **MODIFIED_ROSENBROCK**, **ROSENBROCK**,
  LF_POLY_PROD, **POLY_PROD**, **GERSTNER**, **SCALABLE_GERSTNER**,
  LOGNORMAL_RATIO, **MULTIMODAL**, **PLUGIN_ROSENBROCK**, **PLUGIN_TEXT_BOOK**,
  SHORT_COLUMN, **LF_SHORT_COLUMN**, **MF_SHORT_COLUMN**, **SIDE_IMPACT_COST**,
  SIDE_IMPACT_PERFORMANCE, **SOBOL_RATIONAL**, **SOBOL_G_FUNCTION**, **SOBOL_ISHIGAMI**,
  STEEL_COLUMN_COST, **STEEL_COLUMN_PERFORMANCE**, **TEXT_BOOK**, **TEXT_BOOK1**,
  TEXT_BOOK2, **TEXT_BOOK3**, **TEXT_BOOK_OUU**, **SCALABLE_TEXT_BOOK**,
  SCALABLE_MONOMIALS, **MOGATEST1**, **MOGATEST2**, **MOGATEST3**,
  ILLUMINATION, **BARNES**, **BARNES_LF**, **HERBIE**,
  SMOOTH_HERBIE, **SHUBERT**, **SALINAS**, **MODELCENTER**,
  GENZ, **DAMPED_OSCILLATOR**, **ANISOTROPIC_QUADRATIC_FORM**, **BAYES_LINEAR**,
  STEADY_STATE_DIFFUSION_1D, **SS_DIFFUSION_DISCREPANCY**, **TRANSIENT_DIFFUSION_1D**, **PREDATOR_PREY**,
  PROBLEM18, **TUNABLE_MODEL** }

  enumeration of possible direct driver types (to index to names)
- enum local_data_t { **VARIABLES_MAP** =1, **VARIABLES_VECTOR** =2 }

  enumeration for how local variables are stored (values must employ a bit representation)
- enum sigtype { **NO_SIGMA**, **SCALAR_SIGMA**, **DIAGONAL_SIGMA**, **MATRIX_SIGMA** }

  special values for sigmaType
- enum edtype { **SCALAR_DATA**, **FUNCTIONAL_DATA** }

  special values for experimental data type
- enum {
  DEFAULT_CORRECTION = 0, **SINGLE_CORRECTION**, **FULL_MODEL_FORM_CORRECTION**, **FULL_SOLUTION_LEVEL_CORRECTION**,
  SEQUENCE_CORRECTION }
- enum { **SETUP_MODEL**, **SETUP_USERFUNC** }
- enum {
  CAUVar_normal = 0, **CAUVar_lognormal** = 1, **CAUVar_uniform** = 2, **CAUVar_loguniform** = 3,
  CAUVar_triangular = 4, **CAUVar_exponential** = 5, **CAUVar_beta** = 6, **CAUVar_gamma** = 7,
  CAUVar_gumbel = 8, **CAUVar_frechet** = 9, **CAUVar_weibull** = 10, **CAUVar_histogram_bin** = 11,

CAUVar_Nkinds = 12 }
- enum {
DAUIVar_poisson = 0, **DAUIVar_binomial** = 1, **DAUIVar_negative_binomial** = 2, **DAUIVar_geometric** = 3,
DAUIVar_hypergeometric = 4, **DAUIVar_histogram_point_int** = 5, **DAUIVar_Nkinds** = 6 }
- enum { **DAUSVar_histogram_point_str** = 0, **DAUSVar_Nkinds** = 1 }
- enum { **DAURVar_histogram_point_real** = 0, **DAURVar_Nkinds** = 1 }
- enum { **CEUVar_interval** = 0, **CEUVar_Nkinds** = 1 }
- enum { **DEUIVar_interval** = 0, **DEUIVar_set_int** = 1, **DEUIVar_Nkinds** = 2 }
- enum { **DEUSVar_set_str** = 0, **DEUSVar_Nkinds** = 1 }
- enum { **DEURVar_set_real** = 0, **DEURVar_Nkinds** = 1 }
- enum {
DiscSetVar_design_set_int = 0, **DiscSetVar_design_set_str** = 1, **DiscSetVar_design_set_real** = 2, **Disc-SetVar_state_set_int** = 3,
DiscSetVar_state_set_str = 4, **DiscSetVar_state_set_real** = 5, **DiscSetVar_Nkinds** = 6 }
- enum { **NUM_UNC_REAL_CONT** = 4 }

  number of real-valued uncertain contiguous containers
- enum { **NUM_UNC_INT_CONT** = 2 }

  number of int-valued uncertain contiguous containers
- enum { **NUM_UNC_STR_CONT** = 2 }

  number of string-valued uncertain contiguous containers
- enum **miAlg** : unsigned short { **MI_ALG_KSG1** = 0, **MI_ALG_KSG2** = 1 }
- enum {
ANALYTIC_SOLUTION = 1, **REORDERED_ANALYTIC_SOLUTION**, **R_ONLY_LINEAR_CONSTRAINT**, **N_VECTOR_LINEAR_CONSTRAINT**,
R_AND_N_NONLINEAR_CONSTRAINT }
- enum { **FULL_TENSOR**, **FILTERED_TENSOR**, **RANDOM_TENSOR** }
- enum CG_UPDATETYPE {
CG_STEEPEST, **CG_FLETCHER_REEVES**, **CG_POLAK_RIBIERE**, **CG_POLAK_RIBIERE_PLUS**,
CG_HESTENES_STIEFEL }

  NonlinearCG update options.
- enum CG_LINESEARCHTYPE { **CG_FIXED_STEP**, **CG_LS_SIMPLE**, **CG_LS_BRENT**, **CG_LS_WOLFE** }

  NonlinearCG linesearch options.
- enum { **AS_FUNC** =1, **AS_GRAD** =2, **AS_HESS** =4 }
- enum { **TYPE_U** =1, **TYPE_B** =2, **TYPE_E** =3, **TYPE_EB** =4 }
- enum { **DISALLOW**, **TARGET**, **BOUNDS** }

  to restrict type of auto scaling allowed
- enum { **SCALE_NONE** = 0, **SCALE_VALUE** = 1, **SCALE_LOG** = 2, **SCALE_AUTO** = 4 }

  indicate type of scaling active for a component (bitwise)
- enum EvalType { **NO_EVALUATOR**, **NLF_EVALUATOR**, **CON_EVALUATOR** }

  enumeration for the type of evaluator function
- enum { **APPROX_RESPONSE** =1, **TRUTH_RESPONSE** }
- enum { **CORR_APPROX_RESPONSE** =1, **UNCORR_APPROX_RESPONSE**, **CORR_TRUTH_RESPONS-E**, **UNCORR_TRUTH_RESPONSE** }
- enum {
NEW_CANDIDATE = 1, **CANDIDATE_ACCEPTED** = 2, **CANDIDATE_STATE** = (NEW_CANDIDATE | CA-NDIDATE_ACCEPTED), **NEW_CENTER** = 8,
CENTER_BUILT = 16, **CENTER_STATE** = (NEW_CENTER | CENTER_BUILT), **NEW_TR_FACTOR** = 64,
NEW_TRUST_REGION = (NEW_CENTER | NEW_TR_FACTOR),
HARD_CONVERGED = 128, **SOFT_CONVERGED** = 256, **MIN_TR_CONVERGED** = 512, **MAX_ITER_CO-NVERGED** = 1024,
CONVERGED }
- enum {
TH_SILENT_OUTPUT, **TH_QUIET_OUTPUT**, **TH_NORMAL_OUTPUT**, **TH_VERBOSE_OUTPUT**,
TH_DEBUG_OUTPUT }

- enum { **DIR_CLEAN**, **DIR_PERSIST**, **DIR_ERROR** }

    define directory creation options
- enum { **FILEOP_SILENT**, **FILEOP_WARN**, **FILEOP_ERROR** }

    enum indicating action on failed file operation

Functions

- void **batch_means_interval** (RealMatrix &mcmc_matrix, RealMatrix &interval_matrix, RealMatrix &means_-matrix, int moment, Real alpha)
- void **batch_means_percentile** (RealMatrix &mcmc_matrix, RealMatrix &interval_matrix, RealMatrix &means_matrix, Real percentile, Real alpha)
- CommandShell & flush (CommandShell &shell)

    convenient shell manipulator function to "flush" the shell
- void read_sized_data (std::istream &s, RealVectorArray &va, size_t num_rows, int num_cols)

    istream extraction operator for configuration data of known dim and length
- void read_fixed_rowsize_data (std::istream &s, RealVectorArray &va, int num_cols, bool row_major)

    istream extraction operator for response data of known dim and unknown length
- void read_unsized_data (std::istream &s, RealVectorArray &va, bool row_major)

    istream extraction operator for coordinate data of unknown dim and unknown length
- void **read_config_vars_multifile** (const std::string &basename, int num_expts, int ncv, std::vector< Variables > &config_vars)
- void **read_config_vars_singlefile** (const std::string &basename, int num_expts, int ncv, std::vector< Variables > &config_vars)
- void read_field_values (const std::string &basename, int expt_num, RealVectorArray &field_vars)

    file reader for vector field (response) data
- void read_field_values (const std::string &basename, int expt_num, RealVector &field_vars)

    file reader for scalar field (response) data
- void read_coord_values (const std::string &basename, int expt_num, RealMatrix &coords)

    file reader for experimental coordinate data
- void read_coord_values (const std::string &basename, RealMatrix &coords)

    file reader for simulation coordinate data
- void read_covariance (const std::string &basename, int expt_num, RealMatrix &cov_vals)

    file reader for CONSTANT covariance data
- void read_covariance (const std::string &basename, int expt_num, Dakota::CovarianceMatrix::FORMAT format, int num_vals, RealMatrix &cov_vals)

    file reader for VECTOR and MATRIX covariance data
- bool nearby (const RealVector &rv1, const RealVector &rv2, Real rel_tol)

    tolerance-based equality operator for RealVector
- bool operator== (const ShortArray &dsa1, const ShortArray &dsa2)

    equality operator for ShortArray
- bool operator== (const StringArray &dsa1, const StringArray &dsa2)

    equality operator for StringArray
- Real rel_change_L2 (const RealVector &curr_rv, const RealVector &prev_rv)

    Computes relative change between RealVectors using Euclidean L2 norm.
- Real rel_change_L2 (const RealVector &curr_rv1, const RealVector &prev_rv1, const IntVector &curr_iv, const IntVector &prev_iv, const RealVector &curr_rv2, const RealVector &prev_rv2)

    Computes relative change between Real/int/Real vector triples using Euclidean L2 norm.
- void compute_col_means (RealMatrix &matrix, RealVector &avg_vals)

    Computes means of columns of matrix.
- void compute_col_stdevs (RealMatrix &matrix, RealVector &avg_vals, RealVector &std_devs)

    Computes standard deviations of columns of matrix.

- void remove_column (RealMatrix &matrix, int index)

  Removes column from matrix.
- std::vector< std::string > strsplit (const std::string &input)

  Trim then split a string on {space, tab} and return as vector of strings.
- std::string::size_type longest_strlen (const std::vector< std::string > &vecstr)

  Return the length of the longest string in the passed vector.
- void iround (const RealVector &input_vec, IntVector &rounded_vec)

  round entries of a RealVector yielding an IntVector
- bool operator== (const IntArray &dia1, const IntArray &dia2)

  equality operator for IntArray
- template<typename T >
  bool operator== (const std::vector< T > &vec, typename boost::multi_array< T, 1 >::template const_array-_view< 1 >::type mav)

  equality operator for std::vector and boost::multi_array::const_array_view
- template<typename T >
  bool operator== (typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav, const std::vector< T > &vec)

  equality operator for boost::multi_array::const_array_view and std::vector
- template<typename T >
  bool operator== (const boost::multi_array< T, 1 > &ma, typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav)

  equality operator for boost::multi_array and boost::multi_array::const_array_view
- template<typename T >
  bool operator== (typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav, const boost::multi_array< T, 1 > &ma)

  equality operator for boost::multi_array::const_array_view and boost::multi_array
- bool operator!= (const IntArray &dia1, const IntArray &dia2)

  inequality operator for IntArray
- bool operator!= (const ShortArray &dsa1, const ShortArray &dsa2)

  inequality operator for ShortArray
- bool operator!= (const StringArray &dsa1, const StringArray &dsa2)

  inequality operator for StringArray
- template<typename T >
  bool operator!= (const std::vector< T > &vec, typename boost::multi_array< T, 1 >::template const_array_-view< 1 >::type mav)

  inequality operator for std::vector and boost::multi_array::const_array_view
- template<typename T >
  bool operator!= (typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav, const std::vector< T > &vec)

  inequality operator for boost::multi_array::const_array_view and std::vector
- template<typename T >
  bool operator!= (const boost::multi_array< T, 1 > &ma, typename boost::multi_array< T, 1 >::template const-_array_view< 1 >::type mav)

  inequality operator for boost::multi_array and boost::multi_array::const_array_view
- template<typename T >
  bool operator!= (typename boost::multi_array< T, 1 >::template const_array_view< 1 >::type mav, const boost::multi_array< T, 1 > &ma)

  inequality operator for boost::multi_array::const_array_view and boost::multi_array
- template<typename OrdinalType >
  bool non_zero (const std::vector< OrdinalType > &vec)

  checks for any non-zero value in std::vector(); useful for determining whether an array of request codes (e.g., an ASV) has any actionable content

- template<typename VectorType >
  bool is_equal_vec (const RealVector &vec1, const VectorType &vec2)

  equality function for RealVector and a vector of arbitrary type
- template<typename MatrixType , typename VectorType >
  void apply_matrix_partial (const MatrixType &M, const VectorType &v1, VectorType &v2)

  Applies a RealMatrix to a vector (or subset of vector) v1.
- template<typename VectorType >
  void apply_matrix_transpose_partial (const RealMatrix &M, const VectorType &v1, VectorType &v2)

  Applies transpose of a RealMatrix to a vector (or subset of vector) v1.
- std::string strtolower (const std::string &s)

  Return lowercase copy of string s.
- bool strbegins (const std::string &input, const std::string &test)

  Return true if input string begins with string test.
- bool strends (const std::string &input, const std::string &test)

  Return true if input string ends with string test.
- bool strcontains (const std::string &input, const std::string &test)

  Return true if input string contains string test.
- void build_label (String &label, const String &root_label, size_t tag, const String &separator="")

  create a label by appending a numerical tag to the root_label, o
- void build_labels (StringArray &label_array, const String &root_label)

  create an array of labels by tagging root_label for each entry in label_array. Uses build_label().
- void build_labels (StringMultiArray &label_array, const String &root_label)

  create an array of labels by tagging root_label for each entry in label_array. Uses build_label().
- void build_labels_partial (StringArray &label_array, const String &root_label, size_t start_index, size_t num_-items)

  create a partial array of labels by tagging root_label for a subset of entries in label_array. Uses build_label().
- template<typename vecType , typename valueType >
  void assign_value (vecType &target, valueType val)

  assign a value to an arbitrary vector
- template<typename vecType , typename valueType >
  void assign_value (vecType &target, valueType val, size_t start, size_t len)

  assign a value to a portion of an arbitrary vector
- template<typename OrdinalType , typename ScalarType >
  void copy_data (const std::vector< Teuchos::SerialDenseVector< OrdinalType, ScalarType > > &sdva, Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > &sdm)

  copy Array<Teuchos::SerialDenseVector<OT,ST> > to Teuchos::SerialDenseMatrix<OT,ST> - used by read_data-_tabular - RWH
- template<typename OrdinalType , typename ScalarType >
  void copy_data_transpose (const std::vector< Teuchos::SerialDenseVector< OrdinalType, ScalarType > > &sdva, Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > &sdm)

  copy Array<Teuchos::SerialDenseVector<OT,ST> > to transposed Teuchos::SerialDenseMatrix<OT,ST> - used by read_data_tabular - RWH
- template<typename OrdinalType1 , typename OrdinalType2 , typename ScalarType >
  void copy_data (const Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv, Teuchos::Serial-DenseMatrix< OrdinalType1, ScalarType > &sdm, OrdinalType2 nr, OrdinalType2 nc)

  copy Teuchos::SerialDenseVector<OT,ST> to Teuchos::SerialDenseMatrix<OT,ST> - used by NestedModel-::update_sub_iterator - RWH
- template<typename T >
  void copy_data (const std::vector< std::vector< T > > &d2a, std::vector< T > &da)

  copy std::vector<vector<T> > to std::vector<T>(unroll vecOfvecs into vector) - used by ProcessApplicInterface-::write_parameters_files - RWH
- template<typename T >
  void copy_data (const std::map< int, T > &im, std::vector< T > &da)

copy map<int, T> to std::vector<T> (discard integer keys) - used by SurrBasedGlobalMinimizer::core_run - RWH

- template<typename OrdinalType , typename ScalarType >
  void copy_data (const Teuchos::SerialDenseVector< OrdinalType, ScalarType > &sdv1, Teuchos::SerialDenseVector< OrdinalType, ScalarType > &sdv2)

  copy Teuchos::SerialDenseVector<OrdinalType, ScalarType> to same (used in place of operator= when a deep copy is required) - used by Response - MSE

- template<typename OrdinalType , typename ScalarType >
  void copy_data (const Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > &sdm1, Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > &sdm2)

  copy Teuchos::SerialDenseMatrix<OrdinalType, ScalarType> to same (used in place of operator= when a deep copy is required) - used by Response - MSE

- template<typename OrdinalType , typename ScalarType >
  void copy_data (const Teuchos::SerialSymDenseMatrix< OrdinalType, ScalarType > &ssdm1, Teuchos::SerialSymDenseMatrix< OrdinalType, ScalarType > &ssdm2)

  copy Teuchos::SerialSymDenseMatrix<OrdinalType, ScalarType> to same (used in place of operator= when a deep copy is required) - used by Response - MSE

- void copy_data (const RealMatrix &source, RealMatrix &dest, int num_rows, int num_cols, int start_row=0, int start_col=0)

  Taken from pecos/src/MathTools.hpp, BUT not templated because the implementation is specific to RealMatrix.

- template<typename OrdinalType , typename ScalarType , typename VecType >
  void copy_data (const Teuchos::SerialDenseVector< OrdinalType, ScalarType > &sdv, VecType &vec)

  copy Teuchos::SerialDenseVector<OrdinalType, ScalarType> to VecType - used by APPS for HOPS vector types

- template<typename OrdinalType , typename ScalarType1 , typename ScalarType2 >
  void copy_data (const Teuchos::SerialDenseVector< OrdinalType, ScalarType1 > &sdv, std::vector< ScalarType2 > &vec)

  copy Teuchos::SerialDenseVector<OrdinalType, ScalarType> to std::vector<ScalarType> - used by DakotaModel

- template<typename OrdinalType , typename ScalarType >
  void copy_data (const std::vector< ScalarType > &da, Teuchos::SerialDenseVector< OrdinalType, ScalarType > &sdv)

  copy Array<ScalarType> to Teuchos::SerialDenseVector<OrdinalType, ScalarType> - used by NOWPACOptimizer - MSE

- template<typename OrdinalType1 , typename OrdinalType2 , typename ScalarType >
  void copy_data (const ScalarType *ptr, const OrdinalType2 ptr_len, Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv)

  copy ScalarType to Teuchos::SerialDenseVector<OrdinalType, ScalarType> - used by ScalingModel::response_modify_n2s - RWH*

- template<typename OrdinalType1 , typename OrdinalType2 , typename ScalarType >
  void copy_data (const Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv, ScalarType *ptr, const OrdinalType2 ptr_len)

  copy ScalarType to Teuchos::SerialDenseVector<OrdinalType, ScalarType> - used by NL2SOLLeastSq::core_run - RWH*

- template<typename OrdinalType1 , typename OrdinalType2 , typename ScalarType >
  void copy_data (const Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv, std::vector< Teuchos::SerialDenseVector< OrdinalType1, ScalarType > > &sdva, OrdinalType2 num_vec, OrdinalType2 vec_len)

  copy SerialDenseVector<> to Array<SerialDenseVector<> > - used by ConcurrentMetaIterator constructor - RWH

- template<typename vecType1 , typename vecType2 >
  void copy_data_partial (const vecType1 &source, size_t source_start_idx, vecType2 &target, size_t target_start_idx, size_t len)

  copy a portion arbitrary vector to all of another arbitrary vector

- template<typename OrdinalType1 , typename OrdinalType2 , typename ScalarType >
  void copy_data_partial (const Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv1, OrdinalType2 start_index1, OrdinalType2 num_items, Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv2)

  copy portion of first SerialDenseVector to all of second SerialDenseVector - used by DataTransformModel::vars_mapping - RWH

- template<typename OrdinalType1 , typename OrdinalType2 , typename ScalarType >
  void copy_data_partial (const Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv1, Teuchos::-SerialDenseVector< OrdinalType1, ScalarType > &sdv2, OrdinalType2 start_index2)

  copy all of first SerialDenseVector to portion of second SerialDenseVector - used by MixedVariables - RWH, NLSSO-LLeastSq - BMA
- template<typename OrdinalType1 , typename OrdinalType2 , typename ScalarType >
  void copy_data_partial (const Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv1, Ordinal-Type2 start_index1, OrdinalType2 num_items, Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv2, OrdinalType2 start_index2)

  copy portion of first SerialDenseVector to portion of second SerialDenseVector - used by ScalingModel::secondary_-resp_scaled2native - RWH
- template<typename OrdinalType1 , typename OrdinalType2 , typename ScalarType >
  void copy_data_partial (const Teuchos::SerialDenseVector< OrdinalType1, ScalarType > &sdv1, std-::vector< ScalarType > &da2, OrdinalType2 start_index2)

  copy all of first SerialDenseVector to portion of second SerialDenseVector - used by SharedSurfpackApproxData-::merge_variable_arrays - RWH
- template<typename T >
  void copy_data_partial (const std::vector< T > &da1, size_t start_index1, size_t num_items, std::vector< T > &da2)

  copy portion of first Array<T> to all of second Array<T> - used by SharedResponseDataRep constructor - RWH
- template<typename T >
  void copy_data_partial (const std::vector< T > &da1, std::vector< T > &da2, size_t start_index2)

  copy all of first Array<T> to portion of second Array<T> - used by ParamStudy::multidim_loop - RWH
- template<typename T >
  void copy_data_partial (const std::vector< T > &da, boost::multi_array< T, 1 > &bma, size_t start_index_-bma)

  copy all of first Array<T> to portion of boost::multi_array<T, 1> - used by RelaxedVariables - RWH
- template<typename VectorType >
  void copy_column_vector (const RealMatrix &m, RealMatrix::ordinalType j, VectorType &col)

  Copies a column of a Teuchos_SerialDenseMatrix<int,Real> to std::vector<Real>
- template<typename VectorType >
  void copy_row_vector (const RealMatrix &m, RealMatrix::ordinalType i, VectorType &row)

  Copies a row of a Teuchos_SerialDenseMatrix<int,Real> to std::vector<Real>
- template<typename ScalarType >
  void insert_row_vector (const std::vector< ScalarType > &row, RealMatrix::ordinalType i, RealMatrix &m)

  Inserts a std::vector<Real> into a row of a Teuchos_SerialDenseMatrix<int,Real>
- void merge_data_partial (const IntVector &d_vec, RealVector &m_vec, size_t start_index_ma)

  merge a discrete integer vector into a single continuous vector
- void merge_data_partial (const IntVector &d_vec, RealArray &m_array, size_t start_index_ma)

  merge a discrete integer vector into a single continuous array
- template<typename OrdinalType , typename ScalarType >
  const ScalarType & set_index_to_value (OrdinalType index, const std::set< ScalarType > &values)

  retrieve the set value corresponding to the passed index
- template<typename ScalarType >
  size_t set_value_to_index (const ScalarType &value, const std::set< ScalarType > &values)

  calculate the set index corresponding to the passed value
- template<typename OrdinalType , typename KeyType , typename ValueType >
  const KeyType & map_index_to_key (OrdinalType index, const std::map< KeyType, ValueType > &pairs)

  retrieve the set value corresponding to the passed index
- template<typename OrdinalType , typename KeyType , typename ValueType >
  const ValueType & map_index_to_value (OrdinalType index, const std::map< KeyType, ValueType > &pairs)

  retrieve the set value corresponding to the passed index

- template<typename KeyType , typename ValueType >
  void map_keys_to_set (const std::map< KeyType, ValueType > &source_map, std::set< KeyType > &target-_set)

  calculate the map index corresponding to the passed key
- template<typename KeyType , typename ValueType >
  size_t map_key_to_index (const KeyType &key, const std::map< KeyType, ValueType > &pairs)

  calculate the map index corresponding to the passed key
- template<typename KeyType , typename ValueType >
  size_t map_value_to_index (const ValueType &value, const std::map< KeyType, ValueType > &pairs)

  calculate the map index corresponding to the passed value (not the key)
- template<typename KeyType , typename ValueType >
  size_t map_value_to_index (const ValueType &value, const std::multimap< KeyType, ValueType > &pairs)

  calculate the map index corresponding to the passed value (not the key)
- template<typename OrdinalType , typename ScalarType >
  void x_y_pairs_to_x_set (const Teuchos::SerialDenseVector< OrdinalType, ScalarType > &xy_pairs, std-::set< ScalarType > &x_set)

  convert a SerialDenseVector of head-to-tail (x,y) pairs into a std::set of (x), discarding the y values
- template<typename ScalarType >
  ScalarType **find_min** (const std::vector< ScalarType > &vec)
- template<typename OrdinalType , typename ScalarType >
  ScalarType **find_min** (const std::vector< ScalarType > &vec, OrdinalType start, OrdinalType end)
- template<typename OrdinalType , typename ScalarType >
  ScalarType **find_min** (const Teuchos::SerialDenseVector< OrdinalType, ScalarType > &vec)
- template<typename ScalarType >
  ScalarType **find_min** (const ScalarType ∗vec, size_t len)
- template<typename ScalarType >
  ScalarType **find_max** (const std::vector< ScalarType > &vec)
- template<typename OrdinalType , typename ScalarType >
  ScalarType **find_max** (const Teuchos::SerialDenseVector< OrdinalType, ScalarType > &vec)
- template<typename ContainerType >
  size_t find_index (const ContainerType &c, const typename ContainerType::value_type &search_data)

  generic find_index (inactive)
- template<typename T >
  size_t find_index (const boost::multi_array< T, 1 > &bma, const T &search_data)

  compute the index of an entry within a boost::multi_array
- size_t find_index (SizetMultiArrayConstView bmacv, size_t search_data)

  compute the index of an entry within a boost::multi_array view
- size_t find_index (StringMultiArrayConstView bmacv, const String &search_data)

  compute the index of an entry within a boost::multi_array view
- template<typename ListT >
  size_t find_index (const ListT &l, const typename ListT::value_type &val)

  compute the index of an entry within a std::list
- template<typename ListT >
  ListT::const_iterator find_if (const ListT &c, bool(∗test_fn)(const typename ListT::value_type &, const std-::string &), const std::string &test_fn_data)

  return an iterator to the first list element satisfying the predicate test_fn w.r.t. the passed test_fn_data; end if not found
- template<typename VectorType , typename ScalarType >
  void **copy_data** (const std::vector< VectorType > &va, ScalarType ∗ptr, int ptr_len)
- void copy_data (SizetMultiArrayConstView ma, SizetArray &da)

  copy boost::multi_array view to Array - used by ActiveSet::derivative_vector - RWH
- void copy_data (StringMultiArrayConstView ma, StringArray &da)

  copy boost::multi_array view to Array - used by Pecos::copy_data - RWH
- template<typename DakContainerType >
  bool contains (const DakContainerType &v, const typename DakContainerType::value_type &val)

return true if the item val appears in container v
- void abort_handler (int code)

  global function which handles serial or parallel aborts
- void abort_throw_or_exit (int dakota_code)

  throw or exit depending on abort_mode
- void register_signal_handlers ()

  Tie various signal handlers to Dakota's abort_handler function.
- void mpi_debug_hold ()

  Global function to hold Dakota processes to help with MPI debugging.
- template<typename T >
  T abort_handler_t (int code)
- void svd (RealMatrix &matrix, RealVector &singular_vals, RealMatrix &v_trans, bool compute_vectors=true)

  Compute the SVD of an arbitrary matrix A = USV^T.
- void singular_values (RealMatrix &matrix, RealVector &singular_values)

  compute the singular values without storing any singular vectors (A will be destroyed)
- int qr (RealMatrix &A)

  Compute an in-place QR factorization A = QR.
- int qr_rsolve (const RealMatrix &q_r, bool transpose, RealMatrix &rhs)

  Perform a multiple right-hand sides Rinv ∗ rhs solve using the R from a qr factorization.
- double det_AtransA (RealMatrix &A)

  Use SVD to compute det(A'∗A), destroying A with the SVD.
- std::string string_to_tmpfile (const std::string &dump_string)

  utility to write an input string to a tmpfile in PWD
- std::string pyprepro_input (const std::string &template_file, const std::string &preproc_cmd="pyprepro.py")

  run pyprepro on the user-provided input file and return generated tmp output
- ResultsKeyType make_key (const StrStrSizet &iterator_id, const std::string &data_name)

  Make a full ResultsKeyType from the passed iterator_id and data_name.
- MetaDataValueType make_metadatavalue (StringMultiArrayConstView labels)

  create MetaDataValueType from the passed strings
- MetaDataValueType make_metadatavalue (StringMultiArrayConstView cv_labels, StringMultiArrayConstView div_labels, StringMultiArrayConstView drv_labels, const StringArray &resp_labels)

  create MetaDataValueType from the passed strings
- MetaDataValueType make_metadatavalue (const StringArray &resp_labels)

  create MetaDataValueType from the passed strings
- MetaDataValueType make_metadatavalue (const std::string &)

  create MetaDataValueType from the passed strings
- MetaDataValueType make_metadatavalue (const std::string &, const std::string &)

  create MetaDataValueType from the passed strings
- MetaDataValueType make_metadatavalue (const std::string &, const std::string &, const std::string &)

  create MetaDataValueType from the passed strings
- MetaDataValueType make_metadatavalue (const std::string &, const std::string &, const std::string &, const std::string &)

  create MetaDataValueType from the passed strings
- MetaDataValueType **make_metadatavalue** (StringMultiArrayConstView cv_labels, StringMultiArrayConstView div_labels, StringMultiArrayConstView dsv_labels, StringMultiArrayConstView drv_labels, const StringArray &resp_labels)
- int generate_system_seed ()

  clock microseconds-based random seed in [1, 1000000]
- std::istream & operator>> (std::istream &s, ActiveSet &set)

  std::istream extraction operator for ActiveSet. Calls read(std::istream&).
- std::ostream & operator<< (std::ostream &s, const ActiveSet &set)

std::ostream insertion operator for ActiveSet. Calls write(std::istream&).

- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, ActiveSet &set)

  MPIUnpackBuffer extraction operator for ActiveSet. Calls read(MPIUnpackBuffer&).
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const ActiveSet &set)

  MPIPackBuffer insertion operator for ActiveSet. Calls write(MPIPackBuffer&).
- bool operator!= (const ActiveSet &set1, const ActiveSet &set2)

  inequality operator for ActiveSet
- std::istream & operator>> (std::istream &s, Constraints &con)

  std::istream extraction operator for Constraints
- std::ostream & operator<< (std::ostream &s, const Constraints &con)

  std::ostream insertion operator for Constraints
- std::string re_match (const std::string &token, const boost::regex &re)

  Global utility function to ease migration from CtelRegExp to Boost.Regex.
- bool interface_id_compare (const Interface &interface_in, const void ∗id)

  global comparison function for Interface
- bool method_id_compare (const Iterator &iterator, const void ∗id)

  global comparison function for Iterator
- bool model_id_compare (const Model &model, const void ∗id)

  global comparison function for Model
- bool operator== (const Model &m1, const Model &m2)

  equality operator for Envelope is true if same letter instance
- bool operator!= (const Model &m1, const Model &m2)

  inequality operator for Envelope is true if different letter instance
- template<typename VecT >
  void get_initial_values (const Model &model, VecT &values)
- template<typename VecT >
  bool get_bounds (const RealVector &lower_source, const RealVector &upper_source, VecT &lower_target, VecT &upper_target, Real big_real_bound_size, Real no_value)
- template<typename VecT >
  void get_bounds (const Model &model, VecT &lower_target, VecT &upper_target)
- template<typename SetT , typename VecT >
  void get_bounds (const SetT &source_set, VecT &lower_target, VecT &upper_target, int target_offset)
- template<typename OrdinalType , typename ScalarType , typename VectorType2 , typename MaskType , typename SetArray >
  bool get_mixed_bounds (const MaskType &mask_set, const SetArray &source_set, const Teuchos::SerialDenseVector< OrdinalType, ScalarType > &lower_source, const Teuchos::SerialDenseVector< OrdinalType, ScalarType > &upper_source, VectorType2 &lower_target, VectorType2 &upper_target, ScalarType bigBoundSize, ScalarType no_value, int target_offset=0)
- template<typename AdapterT >
  bool get_variable_bounds (Model &model, Real big_real_bound_size, int big_int_bound_size, typename AdapterT::VecT &lower, typename AdapterT::VecT &upper)
- template<typename RVecT , typename IVecT >
  int configure_inequality_constraint_maps (const Model &model, Real big_real_bound_size, CONSTRAINT_TYPE ctype, IVecT &map_indices, RVecT &map_multipliers, RVecT &map_offsets, Real scaling=1.0)
- template<typename RVecT , typename IVecT >
  void configure_equality_constraint_maps (Model &model, CONSTRAINT_TYPE ctype, IVecT &indices, size_t index_offset, RVecT &multipliers, RVecT &values, bool make_one_sided)
- template<typename AdapterT >
  void get_linear_constraints (Model &model, Real big_real_bound_size, typename AdapterT::VecT &lin_ineq_lower_bnds, typename AdapterT::VecT &lin_ineq_upper_bnds, typename AdapterT::VecT &lin_eq_targets, typename AdapterT::MatT &lin_ineq_coeffs, typename AdapterT::MatT &lin_eq_coeffs)
- template<typename VecT >
  void apply_linear_constraints (const Model &model, CONSTRAINT_EQUALITY_TYPE etype, const VecT &in_vals, VecT &values, bool adjoint=false)

- template<typename VecT >
  void apply_nonlinear_constraints (const Model &model, CONSTRAINT_EQUALITY_TYPE etype, const VecT &in_vals, VecT &values, bool adjoint=false)
- template<typename VectorType1 , typename VectorType2 , typename SetArray >
  void **copy_variables** (const VectorType1 &source, const BitArray &set_bits, const SetArray &set_vars, VectorType2 &dest, size_t offset, size_t len)
- template<typename VectorType1 , typename VectorType2 , typename SetArray >
  void **copy_variables** (const VectorType1 &source, const SetArray &set_vars, VectorType2 &dest, size_t offset, size_t len)
- template<typename VectorType1 , typename VectorType2 >
  void **copy_variables** (const VectorType1 &source, VectorType2 &dest, const BitArray &int_set_bits, const IntSetArray &set_int_vars, size_t offset, size_t len)
- template<typename AdapterT >
  void set_best_responses (typename AdapterT::OptT &optimizer, const Model &model, bool set_objectives, size_t num_user_primary_fns, const std::vector< int > constraint_map_indices, const std::vector< double > constraint_map_multipliers, const std::vector< double > constraint_map_offsets, ResponseArray &response_array)
- template<typename VectorType >
  void set_variables (const VectorType &source, Model &model, Variables &vars)
- template<typename VectorType >
  void get_variables (Model &model, VectorType &vec)
- template<typename vectorType >
  void get_responses (const Model &model, const RealVector &dak_fn_vals, const std::vector< int > constraint_map_indices, const std::vector< double > constraint_map_multipliers, const std::vector< double > constraint_map_offsets, vectorType &f_vec, vectorType &cEqs_vec, vectorType &cIneqs_vec)
- template<typename VecT >
  void get_nonlinear_eq_constraints (const Model &model, VecT &values, Real scale, int offset=-1)
- template<typename VecT >
  void get_nonlinear_eq_constraints (Model &model, const RealVector &curr_resp_vals, VecT &values, Real scale, int offset=0)
- template<typename VecT >
  void get_nonlinear_ineq_constraints (const Model &model, VecT &values)
- template<typename VecT >
  void get_nonlinear_bounds (Model &model, VecT &nonlin_ineq_lower, VecT &nonlin_ineq_upper, VecT &nonlin_eq_targets)

  Would like to combine the previous adapter with this one (based on APPSOptimizer and COLINOptimizer) and then see how much more generalization is needed to support other TPLs like JEGA.
- bool responses_id_compare (const Response &resp, const void *id)

  global comparison function for Response
- std::istream & operator>> (std::istream &s, Response &response)

  std::istream extraction operator for Response. Calls read(std::istream&).
- std::ostream & operator<< (std::ostream &s, const Response &response)

  std::ostream insertion operator for Response. Calls write(std::ostream&).
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, Response &response)

  MPIUnpackBuffer extraction operator for Response. Calls read(MPIUnpackBuffer&).
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const Response &response)

  MPIPackBuffer insertion operator for Response. Calls write(MPIPackBuffer&).
- bool operator!= (const Response &resp1, const Response &resp2)

  inequality operator for Response
- void **set_model_gp_options** (Model &model, const String &options_file)
- bool variables_id_compare (const Variables &vars, const void *id)

  global comparison function for Variables
- std::istream & operator>> (std::istream &s, Variables &vars)

  std::istream extraction operator for Variables.
- std::ostream & operator<< (std::ostream &s, const Variables &vars)

std::ostream insertion operator for Variables.

- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, Variables &vars)

  MPIUnpackBuffer extraction operator for Variables.
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const Variables &vars)

  MPIPackBuffer insertion operator for Variables.
- bool operator!= (const Variables &vars1, const Variables &vars2)

  inequality operator for Variables
- template<typename OrdinalType , typename ScalarType1 , typename ScalarType2 , typename ScalarType3 , typename ScalarType4 >
  void write_ordered (std::ostream &s, const SizetArray &comp_totals, const Teuchos::SerialDenseVector< OrdinalType, ScalarType1 > &c_vector, const Teuchos::SerialDenseVector< OrdinalType, ScalarType2 > &di_vector, const Teuchos::SerialDenseVector< OrdinalType, ScalarType3 > &ds_vector, const Teuchos::SerialDenseVector< OrdinalType, ScalarType4 > &dr_vector)

  free function to write Variables data vectors in input spec ordering
- template<typename OrdinalType , typename ScalarType1 , typename ScalarType2 , typename ScalarType3 , typename ScalarType4 >
  void write_ordered (std::ostream &s, const SizetArray &comp_totals, const Teuchos::SerialDenseVector< OrdinalType, ScalarType1 > &c_vector, const Teuchos::SerialDenseVector< OrdinalType, ScalarType2 > &di_vector, const boost::multi_array< ScalarType3, 1 > &ds_array, const Teuchos::SerialDenseVector< OrdinalType, ScalarType4 > &dr_vector)

  free function to write Variables data vectors in input spec ordering
- template<typename ScalarType >
  void write_ordered (std::ostream &s, const SizetArray &comp_totals, const std::vector< ScalarType > &c_array, const std::vector< ScalarType > &di_array, const std::vector< ScalarType > &ds_array, const std::vector< ScalarType > &dr_array)

  free function to write Variables data vectors in input spec ordering
- void size_and_fill (const SharedVariablesData &svd, size_t array_size, VariablesArray &vars_array)

  Reinitialize var_array to contain array_size freshly constructed Variables, sharing provided SVD.
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const DataEnvironment &data)

  MPIPackBuffer insertion operator for DataEnvironment.
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, DataEnvironment &data)

  MPIUnpackBuffer extraction operator for DataEnvironment.
- std::ostream & operator<< (std::ostream &s, const DataEnvironment &data)

  std::ostream insertion operator for DataEnvironment
- String **interface_enum_to_string** (unsigned short interface_type)
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const DataInterface &data)

  MPIPackBuffer insertion operator for DataInterface.
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, DataInterface &data)

  MPIUnpackBuffer extraction operator for DataInterface.
- std::ostream & operator<< (std::ostream &s, const DataInterface &data)

  std::ostream insertion operator for DataInterface
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const DataMethod &data)

  MPIPackBuffer insertion operator for DataMethod.
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, DataMethod &data)

  MPIUnpackBuffer extraction operator for DataMethod.
- std::ostream & operator<< (std::ostream &s, const DataMethod &data)

  std::ostream insertion operator for DataMethod
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const DataModel &data)

  MPIPackBuffer insertion operator for DataModel.
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, DataModel &data)

  MPIUnpackBuffer extraction operator for DataModel.
- std::ostream & operator<< (std::ostream &s, const DataModel &data)

  std::ostream insertion operator for DataModel
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const DataResponses &data)

MPIPackBuffer insertion operator for DataResponses.
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, DataResponses &data)

  MPIUnpackBuffer extraction operator for DataResponses.
- std::ostream & operator<< (std::ostream &s, const DataResponses &data)

  std::ostream insertion operator for DataResponses
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const DataVariables &data)

  MPIPackBuffer insertion operator for DataVariables.
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, DataVariables &data)

  MPIUnpackBuffer extraction operator for DataVariables.
- std::ostream & operator<< (std::ostream &s, const DataVariables &data)

  std::ostream insertion operator for DataVariables
- int **dlsolver_option** (Opt_Info ∗)
- RealVector const ∗ **continuous_lower_bounds** (Optimizer1 ∗o)
- RealVector const ∗ **continuous_upper_bounds** (Optimizer1 ∗o)
- RealVector const ∗ **nonlinear_ineq_constraint_lower_bounds** (Optimizer1 ∗o)
- RealVector const ∗ **nonlinear_ineq_constraint_upper_bounds** (Optimizer1 ∗o)
- RealVector const ∗ **nonlinear_eq_constraint_targets** (Optimizer1 ∗o)
- RealVector const ∗ **linear_ineq_constraint_lower_bounds** (Optimizer1 ∗o)
- RealVector const ∗ **linear_ineq_constraint_upper_bounds** (Optimizer1 ∗o)
- RealVector const ∗ **linear_eq_constraint_targets** (Optimizer1 ∗o)
- RealMatrix const ∗ **linear_ineq_constraint_coeffs** (Optimizer1 ∗o)
- RealMatrix const ∗ **linear_eq_constraint_coeffs** (Optimizer1 ∗o)
- void **ComputeResponses** (Optimizer1 ∗o, int mode, int n, double ∗x)
- void **GetFuncs** (Optimizer1 ∗o, int m0, int m1, double ∗f)
- void **GetGrads** (Optimizer1 ∗o, int m0, int m1, int n, int is, int js, double ∗g)
- void **GetContVars** (Optimizer1 ∗o, int n, double ∗x)
- void **SetBestContVars** (Optimizer1 ∗o, int n, double ∗x)
- void **SetBestRespFns** (Optimizer1 ∗o, int n, double ∗x)
- void ∗ **dl_constructor** (Optimizer1 ∗, Dakota_funcs ∗, dl_core_run_t ∗, dl_destructor_t ∗)
- static RealVector const ∗ **continuous_lower_bounds1** (Optimizer1 ∗o)
- static RealVector const ∗ **continuous_upper_bounds1** (Optimizer1 ∗o)
- static RealVector const ∗ **nonlinear_ineq_constraint_lower_bounds1** (Optimizer1 ∗o)
- static RealVector const ∗ **nonlinear_ineq_constraint_upper_bounds1** (Optimizer1 ∗o)
- static RealVector const ∗ **nonlinear_eq_constraint_targets1** (Optimizer1 ∗o)
- static RealVector const ∗ **linear_ineq_constraint_lower_bounds1** (Optimizer1 ∗o)
- static RealVector const ∗ **linear_ineq_constraint_upper_bounds1** (Optimizer1 ∗o)
- static RealVector const ∗ **linear_eq_constraint_targets1** (Optimizer1 ∗o)
- static RealMatrix const ∗ **linear_eq_constraint_coeffs1** (Optimizer1 ∗o)
- static RealMatrix const ∗ **linear_ineq_constraint_coeffs1** (Optimizer1 ∗o)
- static void **ComputeResponses1** (Optimizer1 ∗o, int mode, int n, double ∗x)
- static void **GetFuncs1** (Optimizer1 ∗o, int m0, int m1, double ∗f)
- static void **GetGrads1** (Optimizer1 ∗o, int m0, int m1, int n, int is, int js, double ∗g)
- static void **GetContVars1** (Optimizer1 ∗o, int n, double ∗x)
- static void **SetBestContVars1** (Optimizer1 ∗o, int n, double ∗x)
- static void **SetBestDiscVars1** (Optimizer1 ∗o, int n, int ∗x)
- static void **SetBestRespFns1** (Optimizer1 ∗o, int n, double ∗x)
- static double **Get_Real1** (Optimizer1 ∗o, const char ∗name)
- static int **Get_Int1** (Optimizer1 ∗o, const char ∗name)
- static bool **Get_Bool1** (Optimizer1 ∗o, const char ∗name)
- DOTOptimizer ∗ **new_DOTOptimizer** (ProblemDescDB &problem_db)
- DOTOptimizer ∗ **new_DOTOptimizer** (Model &model)
- DOTOptimizer ∗ **new_DOTOptimizer** (ProblemDescDB &problem_db, Model &model)
- void copy_field_data (const RealVector &fn_vals, RealMatrix &fn_grad, const RealSymMatrixArray &fn_hess, size_t offset, size_t num_fns, Response &response)

- void copy_field_data (const RealVector &fn_vals, RealMatrix &fn_grad, const RealSymMatrixArray &fn_hess, size_t offset, size_t num_fns, short total_asv, Response &response)
- void **interpolate_simulation_field_data** (const Response &sim_resp, const RealMatrix &exp_coords, size_t field_num, short total_asv, size_t interp_resp_offset, Response &interp_resp)
- void linear_interpolate_1d (const RealMatrix &build_pts, const RealVector &build_vals, const RealMatrix &build_grads, const RealSymMatrixArray &build_hessians, const RealMatrix &pred_pts, RealVector &pred_-vals, RealMatrix &pred_grads, RealSymMatrixArray &pred_hessians)

  Returns the value of at 1D function f and its gradient and hessians (if available) at the points of vector pred_pts using linear interpolation. The vector build_pts specifies the coordinates of the underlying interval at which the values (build-_vals) of the function f are known. The length of output pred_vals is equal to the length of pred_pts. This function assumes the build_pts is in ascending order.
- void symmetric_eigenvalue_decomposition (const RealSymMatrix &matrix, RealVector &eigenvalues, Real-Matrix &eigenvectors)

  Computes the eigenvalues and, optionally, eigenvectors of a real symmetric matrix A.
- void compute_column_means (RealMatrix &matrix, RealVector &avg_vals)

  Compute the means of each column of an arbitrary matrix.
- void sort_vector (const RealVector &vec, RealVector &sort_vec, IntVector &indices)

  Sort incoming vector with result and corresponding indices returned in passed arguments.
- void sort_matrix_columns (const RealMatrix &mat, RealMatrix &sort_mat, IntMatrix &indices)

  Sort incoming matrix columns with result and corresponding indices returned in passed arguments.
- bool is_matrix_symmetric (const RealMatrix &matrix)

  Test if incoming matrix is symmetric.
- template<typename O , typename T >
  int binary_search (T target, Teuchos::SerialDenseVector< O, T > &data)

  find the interval containing a target value. This function assumes the data is in ascending order.
- Real getdist (const RealVector &x1, const RealVector &x2)
- Real mindist (const RealVector &x, const RealMatrix &xset, int except)
- Real mindistindx (const RealVector &x, const RealMatrix &xset, const IntArray &indx)
- Real getRmax (const RealMatrix &xset)
- int start_grid_computing (char *analysis_driver_script, char *params_file, char *results_file)
- int stop_grid_computing ()
- int perform_analysis (char *iteration_num)
- int length (const StringMultiArrayConstView &vec)

  Return the length of a StringMultiArrayConstView.
- H5::DataType h5_file_dtype (const short &)

  Return the HDF5 datatype to store a short.
- H5::DataType h5_file_dtype (const int &)

  Return the HDF5 datatype to store a int.
- H5::DataType **h5_file_dtype** (const unsigned int &)
- H5::DataType **h5_file_dtype** (const unsigned long &)
- H5::DataType **h5_file_dtype** (const unsigned long long &)
- H5::DataType h5_file_dtype (const Real &)

  Return the HDF5 datatype to store a Real.
- H5::DataType h5_file_dtype (const char *)

  Return the HDF5 datatype to store a string.
- H5::DataType h5_file_dtype (const ResultsOutputType t)

  Overloads for ResultsOutputType (used when creating empty datasets)
- H5::DataType h5_file_dtype (const String &)

  Return the HDF5 datatype to store a string.
- H5::DataType h5_mem_dtype (const Real &)

  Return the HDF5 datatype to read a Real in memory.
- H5::DataType h5_mem_dtype (const short &)

  Return the HDF5 datatype to read a short in memory.

- H5::DataType h5_mem_dtype (const int &)

  Return the HDF5 datatype to read an int in memory.
- H5::DataType h5_mem_dtype (const unsigned int &)

  Return the HDF5 datatype to read an unsigned int in memory.
- H5::DataType h5_mem_dtype (const unsigned long &)

  Return the HDF5 datatype to read an unsigned long (maybe a size_t) in memory.
- H5::DataType h5_mem_dtype (const unsigned long long &)

  Return the HDF5 datatype to read an unsigned long long (maybe a size_t) in memory.
- H5::DataType h5_mem_dtype (const char *)

  Return the HDF5 datatype to read a string in memory.
- H5::DataType h5_mem_dtype (const String &)

  Return the HDF5 datatype to read a string in memory.
- H5::DataType h5_mem_dtype (const ResultsOutputType t)

  Overloads for ResultsOutputType (used when creating empty datasets)
- template<typename T >
  int length (const std::vector< T > &vec)

  Return the length of seeral types.
- template<typename T >
  int length (const Teuchos::SerialDenseVector< int, T > &vec)

  Return the length of an SDV.
- template<typename T >
  std::vector< const char * > pointers_to_strings (const T &data)

  Return a vector of pointers to strings.
- template<typename T >
  string asstring (const T &val)

  Creates a string from the argument val using an ostringstream.
- **PACKBUF** (int, MPI_INT) PACKBUF(u_int
- MPI_UNSIGNED **PACKBUF** (long, MPI_LONG) PACKBUF(u_long
- MPI_UNSIGNED MPI_UNSIGNED_LONG **PACKBUF** (long long, MPI_LONG_LONG) PACKBUF(unsigned long long
- MPI_UNSIGNED MPI_UNSIGNED_LONG
  MPI_UNSIGNED_LONG_LONG **PACKBUF** (short, MPI_SHORT) PACKBUF(u_short
- MPI_UNSIGNED MPI_UNSIGNED_LONG
  MPI_UNSIGNED_LONG_LONG
  MPI_UNSIGNED_SHORT **PACKBUF** (char, MPI_CHAR) PACKBUF(u_char
- MPI_UNSIGNED MPI_UNSIGNED_LONG
  MPI_UNSIGNED_LONG_LONG
  MPI_UNSIGNED_SHORT
  MPI_UNSIGNED_CHAR **PACKBUF** (double, MPI_DOUBLE) PACKBUF(float
- **UNPACKBUF** (int, MPI_INT) UNPACKBUF(u_int
- MPI_UNSIGNED **UNPACKBUF** (long, MPI_LONG) UNPACKBUF(u_long
- MPI_UNSIGNED MPI_UNSIGNED_LONG **UNPACKBUF** (long long, MPI_LONG_LONG) UNPACKBUF(unsigned long long
- MPI_UNSIGNED MPI_UNSIGNED_LONG
  MPI_UNSIGNED_LONG_LONG **UNPACKBUF** (short, MPI_SHORT) UNPACKBUF(u_short
- MPI_UNSIGNED MPI_UNSIGNED_LONG
  MPI_UNSIGNED_LONG_LONG
  MPI_UNSIGNED_SHORT **UNPACKBUF** (char, MPI_CHAR) UNPACKBUF(u_char
- MPI_UNSIGNED MPI_UNSIGNED_LONG
  MPI_UNSIGNED_LONG_LONG
  MPI_UNSIGNED_SHORT
  MPI_UNSIGNED_CHAR **UNPACKBUF** (double, MPI_DOUBLE) UNPACKBUF(float
- **PACKSIZE** (int, MPI_INT) PACKSIZE(u_int
- MPI_UNSIGNED **PACKSIZE** (long, MPI_LONG) PACKSIZE(u_long

- MPI_UNSIGNED MPI_UNSIGNED_LONG **PACKSIZE** (long long, MPI_LONG_LONG) PACKSIZE(unsigned long long
- MPI_UNSIGNED MPI_UNSIGNED_LONG
MPI_UNSIGNED_LONG_LONG **PACKSIZE** (short, MPI_SHORT) PACKSIZE(u_short
- MPI_UNSIGNED MPI_UNSIGNED_LONG
MPI_UNSIGNED_LONG_LONG
MPI_UNSIGNED_SHORT **PACKSIZE** (char, MPI_CHAR) PACKSIZE(u_char
- MPI_UNSIGNED MPI_UNSIGNED_LONG
MPI_UNSIGNED_LONG_LONG
MPI_UNSIGNED_SHORT
MPI_UNSIGNED_CHAR **PACKSIZE** (double, MPI_DOUBLE) PACKSIZE(float
- MPI_UNSIGNED MPI_UNSIGNED_LONG
MPI_UNSIGNED_LONG_LONG
MPI_UNSIGNED_SHORT
MPI_UNSIGNED_CHAR MPI_FLOAT
int MPIPackSize (const bool &data, const int num=1)

    return packed size of a bool
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const int &data)

    insert an int
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const u_int &data)

    insert a u_int
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const long &data)

    insert a long
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const u_long &data)

    insert a u_long
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const long long &data)

    insert a long long
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const unsigned long long &data)

    insert a unsigned long long
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const short &data)

    insert a short
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const u_short &data)

    insert a u_short
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const char &data)

    insert a char
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const u_char &data)

    insert a u_char
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const double &data)

    insert a double
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const float &data)

    insert a float
- MPIPackBuffer & operator<< (MPIPackBuffer &buff, const bool &data)

    insert a bool
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, int &data)

    extract an int
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, u_int &data)

    extract a u_int
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, long &data)

    extract a long
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, u_long &data)

    extract a u_long
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, long long &data)

extract a long long
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, unsigned long long &data)

  extract an unsigned long long
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, short &data)

  extract a short
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, u_short &data)

  extract a u_short
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, char &data)

  extract a char
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, u_char &data)

  extract a u_char
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, double &data)

  extract a double
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, float &data)

  extract a float
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &buff, bool &data)

  extract a bool
- int MPIPackSize (const int &data, const int num=1)

  return packed size of an int
- int MPIPackSize (const u_int &data, const int num=1)

  return packed size of a u_int
- int MPIPackSize (const long &data, const int num=1)

  return packed size of a long
- int MPIPackSize (const u_long &data, const int num=1)

  return packed size of a u_long
- int MPIPackSize (const long long &data, const int num=1)

  return packed size of a long long
- int MPIPackSize (const unsigned long long &data, const int num=1)

  return packed size of an unsigned long long
- int MPIPackSize (const short &data, const int num=1)

  return packed size of a short
- int MPIPackSize (const u_short &data, const int num=1)

  return packed size of a u_short
- int MPIPackSize (const char &data, const int num=1)

  return packed size of a char
- int MPIPackSize (const u_char &data, const int num=1)

  return packed size of a u_char
- int MPIPackSize (const double &data, const int num=1)

  return packed size of a double
- int MPIPackSize (const float &data, const int num=1)

  return packed size of a float
- int **nidr_parse** (const char ∗, FILE ∗)
- const char ∗∗ **arg_list_adjust** (const char ∗∗, void ∗∗)
- int **not_executable** (const char ∗driver_name, const char ∗tdir)
- static void **scale_chk** (StringArray &ST, RealVector &S, const char ∗what, const char ∗∗univ)
- static void **BuildLabels** (StringArray ∗sa, size_t nsa, size_t n1, size_t n2, const char ∗stub)
- static int **mixed_check** (IntSet ∗S, int n, IntArray ∗iv, const char ∗what)
- static void **mixed_check2** (size_t n, IntArray ∗iv, const char ∗what)
- static int **wronglen** (size_t n, RealVector ∗V, const char ∗what)
- static int **wronglen** (size_t n, IntVector ∗V, const char ∗what)
- static void **Vcopyup** (RealVector ∗V, RealVector ∗M, size_t i, size_t n)

- static void **Set_rv** (RealVector ∗V, double d, size_t n)
- static void **Set_iv** (IntVector ∗V, int d, size_t n)
- static void **wrong_number** (const char ∗what, const char ∗kind, size_t nsv, size_t m)
- static void **too_small** (const char ∗kind)
- static void **not_div** (const char ∗kind, size_t nsv, size_t m)
- static void **suppressed** (const char ∗kind, int ndup, int ∗ip, String ∗sp, Real ∗rp)
- static void **bad_initial_ivalue** (const char ∗kind, int val)
- static void **bad_initial_svalue** (const char ∗kind, String val)
- static void **bad_initial_rvalue** (const char ∗kind, Real val)
- static void **Vgen_ContinuousDes** (DataVariablesRep ∗dv, size_t offset)
- static void **Vgen_DiscreteDesRange** (DataVariablesRep ∗dv, size_t offset)
- static void **Vgen_ContinuousState** (DataVariablesRep ∗dv, size_t offset)
- static void **Vgen_DiscreteStateRange** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_NormalUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_NormalUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_LognormalUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_LognormalUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_UniformUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_UniformUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_LoguniformUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_LoguniformUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_TriangularUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_TriangularUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_ExponentialUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_ExponentialUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_BetaUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_BetaUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_GammaUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_GammaUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_GumbelUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_GumbelUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_FrechetUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_FrechetUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_WeibullUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_WeibullUnc** (DataVariablesRep ∗dv, size_t offset)
- static void Vchk_HistogramBinUnc (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)

  Check the histogram bin input data, normalize the counts and populate the histogramUncBinPairs map data structure; map keys are guaranteed unique since the abscissas must increase.
- static void Vgen_HistogramBinUnc (DataVariablesRep ∗dv, size_t offset)

  Infer lower/upper bounds for histogram and set initial variable values based on initial_point or moments, snapping to bounds as needed. (Histogram bin doesn't have lower/upper bounds specifcation)
- static void **Vchk_PoissonUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_PoissonUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_BinomialUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_BinomialUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_NegBinomialUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_NegBinomialUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_GeometricUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_GeometricUnc** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_HyperGeomUnc** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_HyperGeomUnc** (DataVariablesRep ∗dv, size_t offset)
- static void Vchk_HistogramPtIntUnc (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)

  Check the histogram point integer input data, normalize the counts, and populate DataVariables::histogramUncPointIntPairs; map keys are guaranteed unique since the abscissas must increase.

- static void Vgen_HistogramPtIntUnc (DataVariablesRep ∗dv, size_t offset)

  Use the integer-valued point histogram data to initialize the lower, upper, and initial values of the variables, using value closest to mean if no initial point.
- static void Vchk_HistogramPtStrUnc (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)

  Check the histogram point string input data, normalize the counts, and populate DataVariables::histogramUncPoint-StrPairs; map keys are guaranteed unique since the abscissas must increase (lexicographically)
- static void Vgen_HistogramPtStrUnc (DataVariablesRep ∗dv, size_t offset)

  Use the string-valued point histogram data to initialize the lower, upper, and initial values of the variables, using index closest to mean index if no initial point.
- static void Vchk_HistogramPtRealUnc (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)

  Check the histogram point integer real data, normalize the counts, and populate DataVariables::histogramUncPoint-RealPairs; map keys are guaranteed unique since the abscissas must increase.
- static void Vgen_HistogramPtRealUnc (DataVariablesRep ∗dv, size_t offset)

  Use the real-valued point histogram data to initialize the lower, upper, and initial values of the variables, using value closest to mean if no initial point.
- static void Vchk_ContinuousIntervalUnc (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)

  Check the continuous interval uncertain input data and populate DataVariables::continuousIntervalUncBasicProbs; map keys (real intervals) are checked for uniqueness because we don't have a theoretically sound way to combine duplicate intervals.
- static void **Vgen_ContinuousIntervalUnc** (DataVariablesRep ∗dv, size_t offset)
- static void Vchk_DiscreteIntervalUnc (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)

  Check the discrete interval uncertain input data and populate DataVariables::discreteIntervalUncBasicProbs; map keys (integer intervals) are checked for uniqueness because we don't have a theoretically sound way to combine duplicate intervals.
- static void **Vgen_DiscreteIntervalUnc** (DataVariablesRep ∗dv, size_t offset)
- static bool check_set_keys (size_t num_v, size_t ds_len, const char ∗kind, IntArray ∗input_nds, int &avg_-num_ds)

  validate the number of set elements (values) given the number of variables and an optional apportionment with elements_per_variable; return the average number per variable if equally distributed
- static void Vchk_DIset (size_t num_v, const char ∗kind, IntArray ∗input_ndsi, IntVector ∗input_dsi, IntSetArray &dsi_all, IntVector &dsi_init_pt)

  check discrete sets of integers (design and state variables); error if a duplicate value is specified error if not ordered to prevent user confusion
- static void Vchk_DIset (size_t num_v, const char ∗kind, IntArray ∗input_ndsi, IntVector ∗input_dsi, RealVector ∗input_dsip, IntRealMapArray &dsi_vals_probs, IntVector &dsi_init_pt)

  check discrete sets of integers (uncertain variables); error if a duplicate value is specified error if not ordered to prevent user confusion
- static void **Vchk_DSset** (size_t num_v, const char ∗kind, IntArray ∗input_ndss, StringArray ∗input_dss, String-SetArray &dss_all, StringArray &dss_init_pt)
- static void **Vchk_DSset** (size_t num_v, const char ∗kind, IntArray ∗input_ndss, StringArray ∗input_dss, Real-Vector ∗input_dssp, StringRealMapArray &dss_vals_probs, StringArray &dss_init_pt)
- static void **Vchk_DRset** (size_t num_v, const char ∗kind, IntArray ∗input_ndsr, RealVector ∗input_dsr, Real-SetArray &dsr_all, RealVector &dsr_init_pt)
- static void **Vchk_DRset** (size_t num_v, const char ∗kind, IntArray ∗input_ndsr, RealVector ∗input_dsr, Real-Vector ∗input_dsrp, RealRealMapArray &dsr_vals_probs, RealVector &dsr_init_pt)
- static void **Vchk_Adjacency** (size_t num_v, const char ∗kind, const IntArray &num_e, const IntVector &input-_ddsa, RealMatrixArray &dda_all)
- static bool **check_LUV_size** (size_t num_v, IntVector &L, IntVector &U, IntVector &V, bool aggregate_LUV, size_t offset)
- static bool **check_LUV_size** (size_t num_v, StringArray &L, StringArray &U, StringArray &V, bool aggregate-_LUV, size_t offset)
- static bool **check_LUV_size** (size_t num_v, RealVector &L, RealVector &U, RealVector &V, bool aggregate_-LUV, size_t offset)
- template<typename T >
  T midpoint (T a, T b)

Compute the midpoint of floating-point or integer range [a, b] (a <= b), possibly indices, rounding toward a if needed. (Eventually replace with C++20 midpoint, which is more general.)

- static size_t mid_or_next_lower_index (const size_t num_inds)

  get the middle or left-of-middle index among indices [0,num_inds-1]

- static void **Vgen_DIset** (size_t num_v, IntSetArray &sets, IntVector &L, IntVector &U, IntVector &V, bool aggregate_LUV=false, size_t offset=0)
- static void Vgen_DSset (size_t num_v, StringSetArray &sets, StringArray &L, StringArray &U, StringArray &V, bool aggregate_LUV=false, size_t offset=0)

  generate lower, upper, and initial point for string-valued sets

- static void **Vgen_DIset** (size_t num_v, IntRealMapArray &vals_probs, IntVector &IP, IntVector &L, IntVector &U, IntVector &V, bool aggregate_LUV=false, size_t offset=0)
- static void **Vgen_DRset** (size_t num_v, RealSetArray &sets, RealVector &L, RealVector &U, RealVector &V, bool aggregate_LUV=false, size_t offset=0)
- static void **Vgen_DRset** (size_t num_v, RealRealMapArray &vals_probs, RealVector &IP, RealVector &L, RealVector &U, RealVector &V, bool aggregate_LUV=false, size_t offset=0)
- static void **Vgen_DSset** (size_t num_v, StringRealMapArray &vals_probs, StringArray &IP, StringArray &L, StringArray &U, StringArray &V, bool aggregate_LUV=false, size_t offset=0)
- static void **Vchk_DiscreteDesSetInt** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_DiscreteDesSetInt** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_DiscreteDesSetStr** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_DiscreteDesSetStr** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_DiscreteDesSetReal** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_DiscreteDesSetReal** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_DiscreteUncSetInt** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_DiscreteUncSetInt** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_DiscreteUncSetStr** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_DiscreteUncSetStr** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_DiscreteUncSetReal** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_DiscreteUncSetReal** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_DiscreteStateSetInt** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_DiscreteStateSetInt** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_DiscreteStateSetStr** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_DiscreteStateSetStr** (DataVariablesRep ∗dv, size_t offset)
- static void **Vchk_DiscreteStateSetReal** (DataVariablesRep ∗dv, size_t offset, Var_Info ∗vi)
- static void **Vgen_DiscreteStateSetReal** (DataVariablesRep ∗dv, size_t offset)
- static const char ∗ **Var_Name** (StringArray ∗sa, char ∗buf, size_t i)
- static void Var_RealBoundIPCheck (DataVariablesRep ∗dv, Var_rcheck ∗b)

  For real-valued variables: verify lengths of bounds and initial point, validate bounds and adjust initial point to bounds.

- static void Var_IntBoundIPCheck (DataVariablesRep ∗dv, Var_icheck ∗ib)

  For integer-valued variables: verify lengths of bounds and initial point, validate bounds and initial point against bounds.

- static void **flatten_rva** (RealVectorArray ∗rva, RealVector ∗∗prv)
- static void **flatten_iva** (IntVectorArray ∗iva, IntVector ∗∗piv)
- static void **flatten_rsm** (RealSymMatrix ∗rsm, RealVector ∗∗prv)
- static void **flatten_rsa** (RealSetArray ∗rsa, RealVector ∗∗prv)
- static void **flatten_ssa** (StringSetArray ∗ssa, StringArray ∗∗psa)
- static void **flatten_isa** (IntSetArray ∗isa, IntVector ∗∗piv)
- static void **flatten_rrma_keys** (RealRealMapArray ∗rrma, RealVector ∗∗prv)
- static void **flatten_rrma_values** (RealRealMapArray ∗rrma, RealVector ∗∗prv)
- static void **flatten_irma_keys** (IntRealMapArray ∗irma, IntVector ∗∗piv)
- static void **flatten_irma_values** (IntRealMapArray ∗irma, RealVector ∗∗prv)
- static void **flatten_srma_keys** (StringRealMapArray ∗srma, StringArray ∗∗psa)
- static void **flatten_srma_values** (StringRealMapArray ∗srma, RealVector ∗∗prv)
- static void flatten_real_intervals (const RealRealPairRealMapArray &rrprma, RealVector ∗∗probs, RealVector ∗∗lb, RealVector ∗∗ub)

Flatten real-valued interval uncertain variable intervals and probabilities back into separate arrays.

- static void flatten_int_intervals (const IntIntPairRealMapArray &iiprma, RealVector **probs, IntVector **lb, IntVector **ub)

  Flatten integer-valued interval uncertain variable intervals and probabilities back into separate arrays.

- static void **var_iulbl** (const char *keyname, Values *val, VarLabel *vl)
- static Iface_mp_Rlit **MP3** (failAction, recoveryFnVals, recover)
- static Iface_mp_ilit **MP3** (failAction, retryLimit, retry)
- static Iface_mp_lit **MP2** (failAction, abort)
- static Iface_mp_lit **MP2** (failAction, continuation)
- static Iface_mp_type **MP2s** (analysisScheduling, MASTER_SCHEDULING)
- static Iface_mp_type **MP2s** (analysisScheduling, PEER_SCHEDULING)
- static Iface_mp_type **MP2s** (evalScheduling, MASTER_SCHEDULING)
- static Iface_mp_type **MP2s** (evalScheduling, PEER_DYNAMIC_SCHEDULING)
- static Iface_mp_type **MP2s** (evalScheduling, PEER_STATIC_SCHEDULING)
- static Iface_mp_type **MP2s** (asynchLocalEvalScheduling, DYNAMIC_SCHEDULING)
- static Iface_mp_type **MP2s** (asynchLocalEvalScheduling, STATIC_SCHEDULING)
- static Iface_mp_utype **MP2s** (interfaceType, TEST_INTERFACE)
- static Iface_mp_utype **MP2s** (interfaceType, FORK_INTERFACE)
- static Iface_mp_utype **MP2s** (interfaceType, GRID_INTERFACE)
- static Iface_mp_utype **MP2s** (interfaceType, LEGACY_PYTHON_INTERFACE)
- static Iface_mp_utype **MP2s** (interfaceType, MATLAB_INTERFACE)
- static Iface_mp_utype **MP2s** (interfaceType, PLUGIN_INTERFACE)
- static Iface_mp_utype **MP2s** (interfaceType, PYTHON_INTERFACE)
- static Iface_mp_utype **MP2s** (interfaceType, SCILAB_INTERFACE)
- static Iface_mp_utype **MP2s** (interfaceType, SYSTEM_INTERFACE)
- static Iface_mp_utype **MP2s** (resultsFileFormat, LABELED_RESULTS)
- static String **MP_** (algebraicMappings)
- static String **MP_** (idInterface)
- static String **MP_** (inputFilter)
- static String **MP_** (outputFilter)
- static String **MP_** (parametersFile)
- static String **MP_** (pluginLibraryPath)
- static String **MP_** (resultsFile)
- static String **MP_** (workDir)
- static String2DArray **MP_** (analysisComponents)
- static StringArray **MP_** (analysisDrivers)
- static StringArray **MP_** (copyFiles)
- static StringArray **MP_** (linkFiles)
- static bool **MP_** (activeSetVectorFlag)
- static bool **MP_** (allowExistingResultsFlag)
- static bool **MP_** (apreproFlag)
- static bool **MP_** (asynchFlag)
- static bool **MP_** (batchEvalFlag)
- static bool **MP_** (dirSave)
- static bool **MP_** (dirTag)
- static bool **MP_** (evalCacheFlag)
- static bool **MP_** (fileSaveFlag)
- static bool **MP_** (fileTagFlag)
- static bool **MP_** (nearbyEvalCacheFlag)
- static bool **MP_** (numpyFlag)
- static bool **MP_** (restartFileFlag)
- static bool **MP_** (templateReplace)
- static bool **MP_** (useWorkdir)
- static bool **MP_** (verbatimFlag)

- static int **MP_** (analysisServers)
- static int **MP_** (asynchLocalAnalysisConcurrency)
- static int **MP_** (asynchLocalEvalConcurrency)
- static int **MP_** (evalServers)
- static int **MP_** (procsPerAnalysis)
- static int **MP_** (procsPerEval)
- static Real **MP_** (nearbyEvalCacheTol)
- static IntVector **MP_** (primeBase)
- static IntVector **MP_** (refineSamples)
- static IntVector **MP_** (sequenceLeap)
- static IntVector **MP_** (sequenceStart)
- static IntVector **MP_** (stepsPerVariable)
- static Method_mp_ilit2 **MP3** (replacementType, numberRetained, chc)
- static Method_mp_ilit2 **MP3** (replacementType, numberRetained, elitist)
- static Method_mp_ilit2 **MP3** (replacementType, numberRetained, random)
- static Method_mp_ilit2z **MP3** (crossoverType, numCrossPoints, multi_point_binary)
- static Method_mp_ilit2z **MP3** (crossoverType, numCrossPoints, multi_point_parameterized_binary)
- static Method_mp_ilit2z **MP3** (crossoverType, numCrossPoints, multi_point_real)
- static Method_mp_lit **MP2** (batchSelectionType, naive)
- static Method_mp_lit **MP2** (batchSelectionType, distance)
- static Method_mp_lit **MP2** (batchSelectionType, topology)
- static Method_mp_lit **MP2** (batchSelectionType, cl)
- static Method_mp_lit **MP2** (boxDivision, all_dimensions)
- static Method_mp_lit **MP2** (boxDivision, major_dimension)
- static Method_mp_lit **MP2** (convergenceType, average_fitness_tracker)
- static Method_mp_lit **MP2** (convergenceType, best_fitness_tracker)
- static Method_mp_lit **MP2** (convergenceType, metric_tracker)
- static Method_mp_lit **MP2** (crossoverType, blend)
- static Method_mp_lit **MP2** (crossoverType, two_point)
- static Method_mp_lit **MP2** (crossoverType, uniform)
- static Method_mp_lit **MP2** (dataDistCovInputType, diagonal)
- static Method_mp_lit **MP2** (dataDistCovInputType, matrix)
- static Method_mp_lit **MP2** (exploratoryMoves, adaptive)
- static Method_mp_lit **MP2** (exploratoryMoves, multi_step)
- static Method_mp_lit **MP2** (exploratoryMoves, simple)
- static Method_mp_lit **MP2** (fitnessType, domination_count)
- static Method_mp_lit **MP2** (fitnessType, layer_rank)
- static Method_mp_lit **MP2** (fitnessType, linear_rank)
- static Method_mp_lit **MP2** (fitnessType, merit_function)
- static Method_mp_lit **MP2** (fitnessType, proportional)
- static Method_mp_lit **MP2** (fitnessMetricType, predicted_variance)
- static Method_mp_lit **MP2** (fitnessMetricType, distance)
- static Method_mp_lit **MP2** (fitnessMetricType, gradient)
- static Method_mp_lit **MP2** (initializationType, random)
- static Method_mp_lit **MP2** (initializationType, unique_random)
- static Method_mp_lit **MP2** (lipschitzType, global)
- static Method_mp_lit **MP2** (lipschitzType, local)
- static Method_mp_lit **MP2** (meritFunction, merit_max)
- static Method_mp_lit **MP2** (meritFunction, merit_max_smooth)
- static Method_mp_lit **MP2** (meritFunction, merit1)
- static Method_mp_lit **MP2** (meritFunction, merit1_smooth)
- static Method_mp_lit **MP2** (meritFunction, merit2)
- static Method_mp_lit **MP2** (meritFunction, merit2_smooth)
- static Method_mp_lit **MP2** (meritFunction, merit2_squared)
- static Method_mp_lit **MP2** (mcmcType, adaptive_metropolis)

- static Method_mp_lit **MP2** (mcmcType, delayed_rejection)
- static Method_mp_lit **MP2** (mcmcType, dram)
- static Method_mp_lit **MP2** (mcmcType, metropolis_hastings)
- static Method_mp_lit **MP2** (mcmcType, multilevel)
- static Method_mp_lit **MP2** (modelDiscrepancyType, global_kriging)
- static Method_mp_lit **MP2** (modelDiscrepancyType, global_polynomial)
- static Method_mp_lit **MP2** (mutationType, bit_random)
- static Method_mp_lit **MP2** (mutationType, offset_cauchy)
- static Method_mp_lit **MP2** (mutationType, offset_normal)
- static Method_mp_lit **MP2** (mutationType, offset_uniform)
- static Method_mp_lit **MP2** (mutationType, replace_uniform)
- static Method_mp_lit **MP2** (patternBasis, coordinate)
- static Method_mp_lit **MP2** (patternBasis, simplex)
- static Method_mp_lit **MP2** (pointReuse, all)
- static Method_mp_lit **MP2** (proposalCovInputType, diagonal)
- static Method_mp_lit **MP2** (proposalCovInputType, matrix)
- static Method_mp_lit **MP2** (proposalCovType, derivatives)
- static Method_mp_lit **MP2** (proposalCovType, prior)
- static Method_mp_lit **MP2** (proposalCovType, user)
- static Method_mp_lit **MP2** (reliabilityIntegration, first_order)
- static Method_mp_lit **MP2** (reliabilityIntegration, second_order)
- static Method_mp_lit **MP2** (replacementType, elitist)
- static Method_mp_lit **MP2** (replacementType, favor_feasible)
- static Method_mp_lit **MP2** (replacementType, roulette_wheel)
- static Method_mp_lit **MP2** (replacementType, unique_roulette_wheel)
- static Method_mp_lit **MP2** (rngName, mt19937)
- static Method_mp_lit **MP2** (rngName, rnum2)
- static Method_mp_lit **MP2** (searchMethod, gradient_based_line_search)
- static Method_mp_lit **MP2** (searchMethod, tr_pds)
- static Method_mp_lit **MP2** (searchMethod, trust_region)
- static Method_mp_lit **MP2** (searchMethod, value_based_line_search)
- static Method_mp_lit **MP2** (trialType, grid)
- static Method_mp_lit **MP2** (trialType, halton)
- static Method_mp_lit **MP2** (trialType, random)
- static Method_mp_lit **MP2** (useSurrogate, inform_search)
- static Method_mp_lit **MP2** (useSurrogate, optimize)
- static Method_mp_litc **MP3** (crossoverType, crossoverRate, shuffle_random)
- static Method_mp_litc **MP3** (crossoverType, crossoverRate, null_crossover)
- static Method_mp_litc **MP3** (mutationType, mutationRate, null_mutation)
- static Method_mp_litc **MP3** (mutationType, mutationRate, offset_cauchy)
- static Method_mp_litc **MP3** (mutationType, mutationRate, offset_normal)
- static Method_mp_litc **MP3** (mutationType, mutationRate, offset_uniform)
- static Method_mp_litc **MP3** (replacementType, fitnessLimit, below_limit)
- static Method_mp_litrv **MP3** (nichingType, nicheVector, distance)
- static Method_mp_litrv **MP3** (nichingType, nicheVector, max_designs)
- static Method_mp_litrv **MP3** (nichingType, nicheVector, radial)
- static Method_mp_litrv **MP3** (postProcessorType, distanceVector, distance_postprocessor)
- static Method_mp_slit2 **MP3** (initializationType, flatFile, flat_file)
- static Method_mp_utype_lit **MP3s** (methodName, dlDetails, DL_SOLVER)
- static Real **MP_** (absConvTol)
- static Real **MP_** (centeringParam)
- static Real **MP_** (collocationRatio)
- static Real **MP_** (collocRatioTermsOrder)
- static Real **MP_** (constraintPenalty)
- static Real **MP_** (constrPenalty)

- static Real **MP_** (constraintTolerance)
- static Real **MP_** (contractFactor)
- static Real **MP_** (contractStepLength)
- static Real **MP_** (convergenceTolerance)
- static Real **MP_** (crossoverRate)
- static Real **MP_** (falseConvTol)
- static Real **MP_** (functionPrecision)
- static Real **MP_** (globalBalanceParam)
- static Real **MP_** (gradientTolerance)
- static Real **MP_** (hybridLSProb)
- static Real **MP_** (grThreshold)
- static Real **MP_** (initDelta)
- static Real **MP_** (initMeshSize)
- static Real **MP_** (initStepLength)
- static Real **MP_** (initTRRadius)
- static Real **MP_** (lineSearchTolerance)
- static Real **MP_** (localBalanceParam)
- static Real **MP_** (maxBoxSize)
- static Real **MP_** (maxStep)
- static Real **MP_** (minBoxSize)
- static Real **MP_** (minMeshSize)
- static Real **MP_** (multilevEstimatorRate)
- static Real **MP_** (mutationRate)
- static Real **MP_** (mutationScale)
- static Real **MP_** (percentVarianceExplained)
- static Real **MP_** (priorPropCovMult)
- static Real **MP_** (refinementRate)
- static Real **MP_** (regressionL2Penalty)
- static Real **MP_** (shrinkagePercent)
- static Real **MP_** (singConvTol)
- static Real **MP_** (singRadius)
- static Real **MP_** (smoothFactor)
- static Real **MP_** (solnTarget)
- static Real **MP_** (solverRoundingTol)
- static Real **MP_** (solverTol)
- static Real **MP_** (statsRoundingTol)
- static Real **MP_** (stepLenToBoundary)
- static Real **MP_** (threshDelta)
- static Real **MP_** (threshStepLength)
- static Real **MP_** (trustRegionContract)
- static Real **MP_** (trustRegionContractTrigger)
- static Real **MP_** (trustRegionExpand)
- static Real **MP_** (trustRegionExpandTrigger)
- static Real **MP_** (trustRegionMinSize)
- static Real **MP_** (vbdDropTolerance)
- static Real **MP_** (volBoxSize)
- static Real **MP_** (vns)
- static Real **MP_** (wilksConfidenceLevel)
- static Real **MP_** (xConvTol)
- static RealVector **MP_** (anisoDimPref)
- static RealVector **MP_** (concurrentParameterSets)
- static RealVector **MP_** (dataDistCovariance)
- static RealVector **MP_** (dataDistMeans)
- static RealVector **MP_** (finalPoint)
- static RealVector **MP_** (hyperPriorAlphas)

- static RealVector **MP_** (hyperPriorBetas)
- static RealVector **MP_** (listOfPoints)
- static RealVector **MP_** (predictionConfigList)
- static RealVector **MP_** (proposalCovData)
- static RealVector **MP_** (regressionNoiseTol)
- static RealVector **MP_** (scalarizationRespCoeffs)
- static RealVector **MP_** (stepVector)
- static RealVector **MP_** (trustRegionInitSize)
- static RealVectorArray **MP_** (genReliabilityLevels)
- static RealVectorArray **MP_** (probabilityLevels)
- static RealVectorArray **MP_** (reliabilityLevels)
- static RealVectorArray **MP_** (responseLevels)
- static unsigned short **MP_** (adaptedBasisAdvancements)
- static unsigned short **MP_** (cubIntOrder)
- static unsigned short **MP_** (expansionOrder)
- static unsigned short **MP_** (kickOrder)
- static unsigned short **MP_** (maxCVOrderCandidates)
- static unsigned short **MP_** (maxOrder)
- static unsigned short **MP_** (quadratureOrder)
- static unsigned short **MP_** (softConvLimit)
- static unsigned short **MP_** (sparseGridLevel)
- static unsigned short **MP_** (startOrder)
- static unsigned short **MP_** (vbdOrder)
- static unsigned short **MP_** (wilksOrder)
- static SizetArray **MP_** (collocationPointsSeq)
- static SizetArray **MP_** (expansionSamplesSeq)
- static SizetArray **MP_** (pilotSamples)
- static SizetArray **MP_** (randomSeedSeq)
- static SizetArray **MP_** (startRankSeq)
- static UShortArray **MP_** (expansionOrderSeq)
- static UShortArray **MP_** (quadratureOrderSeq)
- static UShortArray **MP_** (sparseGridLevelSeq)
- static UShortArray **MP_** (startOrderSeq)
- static UShortArray **MP_** (tensorGridOrder)
- static UShortArray **MP_** (varPartitions)
- static String **MP_** (advancedOptionsFilename)
- static String **MP_** (betaSolverName)
- static String **MP_** (dataDistFile)
- static String **MP_** (displayFormat)
- static String **MP_** (exportApproxPtsFile)
- static String **MP_** (exportCorrModelFile)
- static String **MP_** (exportCorrVarFile)
- static String **MP_** (exportDiscrepFile)
- static String **MP_** (exportExpansionFile)
- static String **MP_** (exportMCMCPtsFile)
- static String **MP_** (historyFile)
- static String **MP_** (hybridGlobalMethodName)
- static String **MP_** (hybridGlobalMethodPointer)
- static String **MP_** (hybridGlobalModelPointer)
- static String **MP_** (hybridLocalMethodName)
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- static String **MP_** (hybridLocalModelPointer)
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- static String **MP_** (importBuildPtsFile)

- static String **MP_** (importCandPtsFile)
- static String **MP_** (importExpansionFile)
- static String **MP_** (importPredConfigs)
- static String **MP_** (logFile)
- static String **MP_** (lowFidModelPointer)
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- static String **MP_** (posteriorDensityExportFilename)
- static String **MP_** (posteriorSamplesExportFilename)
- static String **MP_** (posteriorSamplesImportFilename)
- static String **MP_** (proposalCovFile)
- static String **MP_** (pstudyFilename)
- static String **MP_** (subMethodName)
- static String **MP_** (subMethodPointer)
- static String **MP_** (subModelPointer)
- static StringArray **MP_** (hybridMethodNames)
- static StringArray **MP_** (hybridMethodPointers)
- static StringArray **MP_** (hybridModelPointers)
- static StringArray **MP_** (miscOptions)
- static bool **MP_** (adaptExpDesign)
- static bool **MP_** (adaptOrder)
- static bool **MP_** (adaptPosteriorRefine)
- static bool **MP_** (adaptRank)
- static bool **MP_** (backfillFlag)
- static bool **MP_** (calModelDiscrepancy)
- static bool **MP_** (chainDiagnostics)
- static bool **MP_** (chainDiagnosticsCI)
- static bool **MP_** (constantPenalty)
- static bool **MP_** (crossValidation)
- static bool **MP_** (crossValidNoiseOnly)
- static bool **MP_** (dOptimal)
- static bool **MP_** (evaluatePosteriorDensity)
- static bool **MP_** (expansionFlag)
- static bool **MP_** (exportSampleSeqFlag)
- static bool **MP_** (exportSurrogate)
- static bool **MP_** (fixedSeedFlag)
- static bool **MP_** (fixedSequenceFlag)
- static bool **MP_** (generatePosteriorSamples)
- static bool **MP_** (gpmsaNormalize)
- static bool **MP_** (importApproxActive)
- static bool **MP_** (importBuildActive)
- static bool **MP_** (latinizeFlag)
- static bool **MP_** (logitTransform)
- static bool **MP_** (mainEffectsFlag)
- static bool **MP_** (methodScaling)
- static bool **MP_** (methodUseDerivsFlag)
- static bool **MP_** (modelEvidence)
- static bool **MP_** (modelEvidLaplace)
- static bool **MP_** (modelEvidMC)
- static bool **MP_** (mutualInfoKSG2)
- static bool **MP_** (mutationAdaptive)
- static bool **MP_** (normalizedCoeffs)
- static bool **MP_** (pcaFlag)
- static bool **MP_** (posteriorStatsKL)
- static bool **MP_** (posteriorStatsKDE)

- static bool **MP_** (posteriorStatsMutual)
- static bool **MP_** (printPopFlag)
- static bool **MP_** (pstudyFileActive)
- static bool **MP_** (randomizeOrderFlag)
- static bool **MP_** (regressDiag)
- static bool **MP_** (relativeConvMetric)
- static bool **MP_** (respScalingFlag)
- static bool **MP_** (showAllEval)
- static bool **MP_** (showMiscOptions)
- static bool **MP_** (speculativeFlag)
- static bool **MP_** (standardizedSpace)
- static bool **MP_** (useTargetVarianceOptimizationFlag)
- static bool **MP_** (tensorGridFlag)
- static bool **MP_** (surrBasedGlobalReplacePts)
- static bool **MP_** (surrBasedLocalLayerBypass)
- static bool **MP_** (truthPilotConstraint)
- static bool **MP_** (vbdFlag)
- static bool **MP_** (volQualityFlag)
- static bool **MP_** (wilksFlag)
- static short **MP_** (polynomialOrder)
- static int **MP_** (batchSize)
- static int **MP_** (batchSizeExplore)
- static int **MP_** (buildSamples)
- static int **MP_** (burnInSamples)
- static int **MP_** (chainSamples)
- static int **MP_** (concurrentRandomJobs)
- static int **MP_** (contractAfterFail)
- static int **MP_** (covarianceType)
- static int **MP_** (crossoverChainPairs)
- static int **MP_** (emulatorOrder)
- static int **MP_** (expandAfterSuccess)
- static int **MP_** (evidenceSamples)
- static int **MP_** (iteratorServers)
- static int **MP_** (jumpStep)
- static int **MP_** (maxCrossIterations)
- static int **MP_** (maxHifiEvals)
- static int **MP_** (mutationRange)
- static int **MP_** (neighborOrder)
- static int **MP_** (newSolnsGenerated)
- static int **MP_** (numChains)
- static int **MP_** (numCR)
- static int **MP_** (numSamples)
- static int **MP_** (numSteps)
- static int **MP_** (numSymbols)
- static int **MP_** (numTrials)
- static int **MP_** (populationSize)
- static int **MP_** (procsPerIterator)
- static int **MP_** (proposalCovUpdatePeriod)
- static int **MP_** (numPushforwardSamples)
- static int **MP_** (randomSeed)
- static int **MP_** (samplesOnEmulator)
- static int **MP_** (searchSchemeSize)
- static int **MP_** (subSamplingPeriod)
- static int **MP_** (totalPatternSize)
- static int **MP_** (verifyLevel)

- static size_t **MP_** (collocationPoints)
- static size_t **MP_** (expansionSamples)
- static size_t **MP_** (kickRank)
- static size_t **MP_** (maxCVRankCandidates)
- static size_t **MP_** (maxFunctionEvals)
- static size_t **MP_** (maxIterations)
- static size_t **MP_** (maxRank)
- static size_t **MP_** (maxRefineIterations)
- static size_t **MP_** (maxSolverIterations)
- static size_t **MP_** (numCandidateDesigns)
- static size_t **MP_** (numCandidates)
- static size_t **MP_** (numDesigns)
- static size_t **MP_** (numFinalSolutions)
- static size_t **MP_** (numGenerations)
- static size_t **MP_** (numOffspring)
- static size_t **MP_** (numParents)
- static size_t **MP_** (numPredConfigs)
- static size_t **MP_** (startRank)
- static Method_mp_type **MP2s** (allocationTarget, TARGET_MEAN)
- static Method_mp_type **MP2s** (allocationTarget, TARGET_SCALARIZATION)
- static Method_mp_type **MP2s** (allocationTarget, TARGET_SIGMA)
- static Method_mp_type **MP2s** (allocationTarget, TARGET_VARIANCE)
- static Method_mp_type **MP2s** (c3AdvanceType, MAX_ORDER_ADVANCEMENT)
- static Method_mp_type **MP2s** (c3AdvanceType, MAX_RANK_ADVANCEMENT)
- static Method_mp_type **MP2s** (c3AdvanceType, MAX_RANK_ORDER_ADVANCEMENT)
- static Method_mp_type **MP2s** (c3AdvanceType, START_ORDER_ADVANCEMENT)
- static Method_mp_type **MP2s** (c3AdvanceType, START_RANK_ADVANCEMENT)
- static Method_mp_type **MP2s** (convergenceToleranceTarget, CONVERGENCE_TOLERANCE_TARGET_C-OST_CONSTRAINT)
- static Method_mp_type **MP2s** (convergenceToleranceTarget, CONVERGENCE_TOLERANCE_TARGET_V-ARIANCE_CONSTRAINT)
- static Method_mp_type **MP2s** (convergenceToleranceType, CONVERGENCE_TOLERANCE_TYPE_ABSO-LUTE)
- static Method_mp_type **MP2s** (convergenceToleranceType, CONVERGENCE_TOLERANCE_TYPE_RELA-TIVE)
- static Method_mp_type **MP2s** (covarianceControl, DIAGONAL_COVARIANCE)
- static Method_mp_type **MP2s** (covarianceControl, FULL_COVARIANCE)
- static Method_mp_type **MP2s** (distributionType, COMPLEMENTARY)
- static Method_mp_type **MP2s** (distributionType, CUMULATIVE)
- static Method_mp_type **MP2s** (emulatorType, EXPGP_EMULATOR)
- static Method_mp_type **MP2s** (emulatorType, GP_EMULATOR)
- static Method_mp_type **MP2s** (emulatorType, KRIGING_EMULATOR)
- static Method_mp_type **MP2s** (emulatorType, MF_PCE_EMULATOR)
- static Method_mp_type **MP2s** (emulatorType, MF_SC_EMULATOR)
- static Method_mp_type **MP2s** (emulatorType, ML_PCE_EMULATOR)
- static Method_mp_type **MP2s** (emulatorType, PCE_EMULATOR)
- static Method_mp_type **MP2s** (emulatorType, SC_EMULATOR)
- static Method_mp_type **MP2s** (emulatorType, VPS_EMULATOR)
- static Method_mp_type **MP2s** (ensembleSampSolnMode, OFFLINE_PILOT)
- static Method_mp_type **MP2s** (ensembleSampSolnMode, ONLINE_PILOT)
- static Method_mp_type **MP2s** (ensembleSampSolnMode, PILOT_PROJECTION)
- static Method_mp_type **MP2s** (evalSynchronize, BLOCKING_SYNCHRONIZATION)
- static Method_mp_type **MP2s** (evalSynchronize, NONBLOCKING_SYNCHRONIZATION)
- static Method_mp_type **MP2p** (expansionBasisType, ADAPTED_BASIS_EXPANDING_FRONT)
- static Method_mp_type **MP2p** (expansionBasisType, ADAPTED_BASIS_GENERALIZED)

- static Method_mp_type **MP2p** (expansionBasisType, HIERARCHICAL_INTERPOLANT)
- static Method_mp_type **MP2p** (expansionBasisType, NODAL_INTERPOLANT)
- static Method_mp_type **MP2p** (expansionBasisType, TENSOR_PRODUCT_BASIS)
- static Method_mp_type **MP2p** (expansionBasisType, TOTAL_ORDER_BASIS)
- static Method_mp_type **MP2s** (expansionType, ASKEY_U)
- static Method_mp_type **MP2s** (expansionType, STD_NORMAL_U)
- static Method_mp_type **MP2p** (finalMomentsType, CENTRAL_MOMENTS)
- static Method_mp_type **MP2p** (finalMomentsType, NO_MOMENTS)
- static Method_mp_type **MP2p** (finalMomentsType, STANDARD_MOMENTS)
- static Method_mp_type **MP2s** (finalStatsType, ESTIMATOR_PERFORMANCE)
- static Method_mp_type **MP2s** (finalStatsType, NO_FINAL_STATS)
- static Method_mp_type **MP2s** (finalStatsType, QOI_STATISTICS)
- static Method_mp_type **MP2p** (growthOverride, RESTRICTED)
- static Method_mp_type **MP2p** (growthOverride, UNRESTRICTED)
- static Method_mp_type **MP2s** (iteratorScheduling, MASTER_SCHEDULING)
- static Method_mp_type **MP2s** (iteratorScheduling, PEER_SCHEDULING)
- static Method_mp_type **MP2s** (lsRegressionType, EQ_CON_LS)
- static Method_mp_type **MP2s** (lsRegressionType, SVD_LS)
- static Method_mp_type **MP2o** (meritFn, ArgaezTapia)
- static Method_mp_type **MP2o** (meritFn, NormFmu)
- static Method_mp_type **MP2o** (meritFn, VanShanno)
- static Method_mp_type **MP2s** (methodOutput, DEBUG_OUTPUT)
- static Method_mp_type **MP2s** (methodOutput, NORMAL_OUTPUT)
- static Method_mp_type **MP2s** (methodOutput, QUIET_OUTPUT)
- static Method_mp_type **MP2s** (methodOutput, SILENT_OUTPUT)
- static Method_mp_type **MP2s** (methodOutput, VERBOSE_OUTPUT)
- static Method_mp_type **MP2s** (multilevAllocControl, ESTIMATOR_VARIANCE)
- static Method_mp_type **MP2s** (multilevAllocControl, GREEDY_REFINEMENT)
- static Method_mp_type **MP2s** (multilevAllocControl, RANK_SAMPLING)
- static Method_mp_type **MP2s** (multilevAllocControl, RIP_SAMPLING)
- static Method_mp_type **MP2s** (multilevDiscrepEmulation, DISTINCT_EMULATION)
- static Method_mp_type **MP2s** (multilevDiscrepEmulation, RECURSIVE_EMULATION)
- static Method_mp_type **MP2p** (nestingOverride, NESTED)
- static Method_mp_type **MP2p** (nestingOverride, NON_NESTED)
- static Method_mp_type **MP2s** (qoiAggregation, QOI_AGGREGATION_MAX)
- static Method_mp_type **MP2s** (qoiAggregation, QOI_AGGREGATION_SUM)
- static Method_mp_type **MP2p** (refinementControl, DIMENSION_ADAPTIVE_CONTROL_GENERALIZED)
- static Method_mp_type **MP2p** (refinementControl, DIMENSION_ADAPTIVE_CONTROL_DECAY)
- static Method_mp_type **MP2p** (refinementControl, DIMENSION_ADAPTIVE_CONTROL_SOBOL)
- static Method_mp_type **MP2p** (refinementControl, LOCAL_ADAPTIVE_CONTROL)
- static Method_mp_type **MP2p** (refinementControl, UNIFORM_CONTROL)
- static Method_mp_type **MP2p** (refinementType, P_REFINEMENT)
- static Method_mp_type **MP2p** (refinementType, H_REFINEMENT)
- static Method_mp_type **MP2p** (regressionType, BASIS_PURSUIT)
- static Method_mp_type **MP2p** (regressionType, BASIS_PURSUIT_DENOISING)
- static Method_mp_type **MP2p** (regressionType, DEFAULT_LEAST_SQ_REGRESSION)
- static Method_mp_type **MP2p** (regressionType, LASSO_REGRESSION)
- static Method_mp_type **MP2p** (regressionType, LEAST_ANGLE_REGRESSION)
- static Method_mp_type **MP2p** (regressionType, ORTHOG_LEAST_INTERPOLATION)
- static Method_mp_type **MP2p** (regressionType, ORTHOG_MATCH_PURSUIT)
- static Method_mp_type **MP2s** (regressionType, FT_LS)
- static Method_mp_type **MP2s** (regressionType, FT_RLS2)
- static Method_mp_type **MP2s** (responseLevelTarget, GEN_RELIABILITIES)
- static Method_mp_type **MP2s** (responseLevelTarget, PROBABILITIES)
- static Method_mp_type **MP2s** (responseLevelTarget, RELIABILITIES)

- static Method_mp_type **MP2s** (responseLevelTargetReduce, SYSTEM_PARALLEL)
- static Method_mp_type **MP2s** (responseLevelTargetReduce, SYSTEM_SERIES)
- static Method_mp_type **MP2p** (statsMetricMode, ACTIVE_EXPANSION_STATS)
- static Method_mp_type **MP2p** (statsMetricMode, COMBINED_EXPANSION_STATS)
- static Method_mp_type **MP2s** (surrBasedLocalAcceptLogic, FILTER)
- static Method_mp_type **MP2s** (surrBasedLocalAcceptLogic, TR_RATIO)
- static Method_mp_type **MP2s** (surrBasedLocalConstrRelax, HOMOTOPY)
- static Method_mp_type **MP2s** (surrBasedLocalMeritFn, ADAPTIVE_PENALTY_MERIT)
- static Method_mp_type **MP2s** (surrBasedLocalMeritFn, AUGMENTED_LAGRANGIAN_MERIT)
- static Method_mp_type **MP2s** (surrBasedLocalMeritFn, LAGRANGIAN_MERIT)
- static Method_mp_type **MP2s** (surrBasedLocalMeritFn, PENALTY_MERIT)
- static Method_mp_type **MP2s** (surrBasedLocalSubProbCon, LINEARIZED_CONSTRAINTS)
- static Method_mp_type **MP2s** (surrBasedLocalSubProbCon, NO_CONSTRAINTS)
- static Method_mp_type **MP2s** (surrBasedLocalSubProbCon, ORIGINAL_CONSTRAINTS)
- static Method_mp_type **MP2s** (surrBasedLocalSubProbObj, AUGMENTED_LAGRANGIAN_OBJECTIVE)
- static Method_mp_type **MP2s** (surrBasedLocalSubProbObj, LAGRANGIAN_OBJECTIVE)
- static Method_mp_type **MP2s** (surrBasedLocalSubProbObj, ORIGINAL_PRIMARY)
- static Method_mp_type **MP2s** (surrBasedLocalSubProbObj, SINGLE_OBJECTIVE)
- static Method_mp_type **MP2s** (wilksSidedInterval, ONE_SIDED_LOWER)
- static Method_mp_type **MP2s** (wilksSidedInterval, ONE_SIDED_UPPER)
- static Method_mp_type **MP2s** (wilksSidedInterval, TWO_SIDED)
- static Method_mp_utype **MP2s** (calibrateErrorMode, CALIBRATE_ONE)
- static Method_mp_utype **MP2s** (calibrateErrorMode, CALIBRATE_PER_EXPER)
- static Method_mp_utype **MP2s** (calibrateErrorMode, CALIBRATE_PER_RESP)
- static Method_mp_utype **MP2s** (calibrateErrorMode, CALIBRATE_BOTH)
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- static Method_mp_utype **MP2s** (importApproxFormat, TABULAR_IFACE_ID)
- static Method_mp_utype **MP2s** (importApproxFormat, TABULAR_ANNOTATED)

- static Method_mp_utype **MP2s** (importBuildFormat, TABULAR_NONE)
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- static Method_mp_utype **MP2s** (integrationRefine, AIS)
- static Method_mp_utype **MP2s** (integrationRefine, IS)
- static Method_mp_utype **MP2s** (integrationRefine, MMAIS)
- static Method_mp_utype **MP2s** (methodName, APPROXIMATE_CONTROL_VARIATE)
- static Method_mp_utype **MP2s** (methodName, ASYNCH_PATTERN_SEARCH)
- static Method_mp_utype **MP2s** (methodName, BRANCH_AND_BOUND)
- static Method_mp_utype **MP2s** (methodName, C3_FUNCTION_TRAIN)
- static Method_mp_utype **MP2s** (methodName, COLINY_BETA)
- static Method_mp_utype **MP2s** (methodName, COLINY_COBYLA)
- static Method_mp_utype **MP2s** (methodName, COLINY_DIRECT)
- static Method_mp_utype **MP2s** (methodName, COLINY_EA)
- static Method_mp_utype **MP2s** (methodName, COLINY_PATTERN_SEARCH)
- static Method_mp_utype **MP2s** (methodName, COLINY_SOLIS_WETS)
- static Method_mp_utype **MP2s** (methodName, CONMIN_FRCG)
- static Method_mp_utype **MP2s** (methodName, CONMIN_MFD)
- static Method_mp_utype **MP2s** (methodName, DACE)
- static Method_mp_utype **MP2s** (methodName, DATA_FIT_SURROGATE_BASED_LOCAL)
- static Method_mp_utype **MP2s** (methodName, DOT_BFGS)
- static Method_mp_utype **MP2s** (methodName, DOT_FRCG)
- static Method_mp_utype **MP2s** (methodName, DOT_MMFD)
- static Method_mp_utype **MP2s** (methodName, DOT_SLP)
- static Method_mp_utype **MP2s** (methodName, DOT_SQP)
- static Method_mp_utype **MP2s** (methodName, EFFICIENT_GLOBAL)
- static Method_mp_utype **MP2s** (methodName, FSU_CVT)
- static Method_mp_utype **MP2s** (methodName, FSU_HALTON)
- static Method_mp_utype **MP2s** (methodName, FSU_HAMMERSLEY)
- static Method_mp_utype **MP2s** (methodName, HIERARCH_SURROGATE_BASED_LOCAL)
- static Method_mp_utype **MP2s** (methodName, HYBRID)
- static Method_mp_utype **MP2s** (methodName, MESH_ADAPTIVE_SEARCH)
- static Method_mp_utype **MP2s** (methodName, MOGA)
- static Method_mp_utype **MP2s** (methodName, MULTI_START)
- static Method_mp_utype **MP2s** (methodName, NCSU_DIRECT)
- static Method_mp_utype **MP2s** (methodName, ROL)
- static Method_mp_utype **MP2s** (methodName, DEMO_TPL)
- static Method_mp_utype **MP2s** (methodName, NL2SOL)
- static Method_mp_utype **MP2s** (methodName, NLPQL_SQP)
- static Method_mp_utype **MP2s** (methodName, NLSSOL_SQP)
- static Method_mp_utype **MP2s** (methodName, MIT_NOWPAC)
- static Method_mp_utype **MP2s** (methodName, MIT_SNOWPAC)
- static Method_mp_utype **MP2s** (methodName, ADAPTIVE_SAMPLING)

- static Method_mp_utype **MP2s** (methodName, BAYES_CALIBRATION)
- static Method_mp_utype **MP2s** (methodName, GENIE_DIRECT)
- static Method_mp_utype **MP2s** (methodName, GENIE_OPT_DARTS)
- static Method_mp_utype **MP2s** (methodName, GPAIS)
- static Method_mp_utype **MP2s** (methodName, GLOBAL_EVIDENCE)
- static Method_mp_utype **MP2s** (methodName, GLOBAL_INTERVAL_EST)
- static Method_mp_utype **MP2s** (methodName, GLOBAL_RELIABILITY)
- static Method_mp_utype **MP2s** (methodName, IMPORTANCE_SAMPLING)
- static Method_mp_utype **MP2s** (methodName, LOCAL_EVIDENCE)
- static Method_mp_utype **MP2s** (methodName, LOCAL_INTERVAL_EST)
- static Method_mp_utype **MP2s** (methodName, LOCAL_RELIABILITY)
- static Method_mp_utype **MP2s** (methodName, MULTIFIDELITY_FUNCTION_TRAIN)
- static Method_mp_utype **MP2s** (methodName, MULTIFIDELITY_POLYNOMIAL_CHAOS)
- static Method_mp_utype **MP2s** (methodName, MULTIFIDELITY_SAMPLING)
- static Method_mp_utype **MP2s** (methodName, MULTIFIDELITY_STOCH_COLLOCATION)
- static Method_mp_utype **MP2s** (methodName, MULTILEVEL_FUNCTION_TRAIN)
- static Method_mp_utype **MP2s** (methodName, MULTILEVEL_MULTIFIDELITY_SAMPLING)
- static Method_mp_utype **MP2s** (methodName, MULTILEVEL_POLYNOMIAL_CHAOS)
- static Method_mp_utype **MP2s** (methodName, MULTILEVEL_SAMPLING)
- static Method_mp_utype **MP2s** (methodName, POF_DARTS)
- static Method_mp_utype **MP2s** (methodName, RKD_DARTS)
- static Method_mp_utype **MP2s** (methodName, POLYNOMIAL_CHAOS)
- static Method_mp_utype **MP2s** (methodName, STOCH_COLLOCATION)
- static Method_mp_utype **MP2s** (methodName, SURROGATE_BASED_UQ)
- static Method_mp_utype **MP2s** (methodName, RANDOM_SAMPLING)
- static Method_mp_utype **MP2s** (methodName, NONLINEAR_CG)
- static Method_mp_utype **MP2s** (methodName, NPSOL_SQP)
- static Method_mp_utype **MP2s** (methodName, OPTPP_CG)
- static Method_mp_utype **MP2s** (methodName, OPTPP_FD_NEWTON)
- static Method_mp_utype **MP2s** (methodName, OPTPP_G_NEWTON)
- static Method_mp_utype **MP2s** (methodName, OPTPP_NEWTON)
- static Method_mp_utype **MP2s** (methodName, OPTPP_PDS)
- static Method_mp_utype **MP2s** (methodName, OPTPP_Q_NEWTON)
- static Method_mp_utype **MP2s** (methodName, PARETO_SET)
- static Method_mp_utype **MP2s** (methodName, PSUADE_MOAT)
- static Method_mp_utype **MP2s** (methodName, RICHARDSON_EXTRAP)
- static Method_mp_utype **MP2s** (methodName, SOGA)
- static Method_mp_utype **MP2s** (methodName, SURROGATE_BASED_GLOBAL)
- static Method_mp_utype **MP2s** (methodName, SURROGATE_BASED_LOCAL)
- static Method_mp_utype **MP2s** (methodName, VECTOR_PARAMETER_STUDY)
- static Method_mp_utype **MP2s** (methodName, LIST_PARAMETER_STUDY)
- static Method_mp_utype **MP2s** (methodName, CENTERED_PARAMETER_STUDY)
- static Method_mp_utype **MP2s** (methodName, MULTIDIM_PARAMETER_STUDY)
- static Method_mp_utype **MP2s** (modelExportFormat, TEXT_ARCHIVE)
- static Method_mp_utype **MP2s** (modelExportFormat, BINARY_ARCHIVE)
- static Method_mp_utype **MP2s** (numericalSolveMode, NUMERICAL_FALLBACK)
- static Method_mp_utype **MP2s** (numericalSolveMode, NUMERICAL_OVERRIDE)
- static Method_mp_utype **MP2s** (optSubProbSolver, SUBMETHOD_NONE)
- static Method_mp_utype **MP2s** (optSubProbSolver, SUBMETHOD_OPTPP)
- static Method_mp_utype **MP2s** (optSubProbSolver, SUBMETHOD_NPSOL)
- static Method_mp_utype **MP2s** (optSubProbSolver, SUBMETHOD_SBLO)
- static Method_mp_utype **MP2s** (optSubProbSolver, SUBMETHOD_EA)
- static Method_mp_utype **MP2s** (optSubProbSolver, SUBMETHOD_EGO)
- static Method_mp_utype **MP2s** (optSubProbSolver, SUBMETHOD_SBGO)
- static Method_mp_utype **MP2s** (optSubProbSolver, SUBMETHOD_LHS)

- static Method_mp_utype **MP2s** (pstudyFileFormat, TABULAR_NONE)
- static Method_mp_utype **MP2s** (pstudyFileFormat, TABULAR_HEADER)
- static Method_mp_utype **MP2s** (pstudyFileFormat, TABULAR_EVAL_ID)
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- static Method_mp_utype **MP2s** (sampleType, SUBMETHOD_LHS)
- static Method_mp_utype **MP2s** (sampleType, SUBMETHOD_RANDOM)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_AMV_PLUS_U)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_AMV_PLUS_X)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_AMV_U)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_AMV_X)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_QMEA_U)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_QMEA_X)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_TANA_U)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_TANA_X)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_NO_APPROX)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_EGRA_U)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_EGRA_X)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_ACV_IS)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_ACV_KL)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_ACV_MF)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_COLLABORATIVE)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_EMBEDDED)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_SEQUENTIAL)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_MUQ)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_DREAM)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_WASABI)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_GPMSA)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_QUESO)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_LHS)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_RANDOM)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_OA_LHS)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_OAS)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_BOX_BEHNKEN)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_CENTRAL_COMPOSITE)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_GRID)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_CONVERGE_ORDER)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_CONVERGE_QOI)
- static Method_mp_utype **MP2s** (subMethod, SUBMETHOD_ESTIMATE_ORDER)
- static SizetSet **MP_** (surrogateFnIndices)
- static Model_mp_lit **MP2** (approxPointReuse, all)
- static Model_mp_lit **MP2** (approxPointReuse, none)
- static Model_mp_lit **MP2** (approxPointReuse, region)
- static Model_mp_lit **MP2** (marsInterpolation, linear)
- static Model_mp_lit **MP2** (marsInterpolation, cubic)
- static Model_mp_lit **MP2** (modelType, active_subspace)
- static Model_mp_lit **MP2** (modelType, adapted_basis)
- static Model_mp_lit **MP2** (modelType, nested)
- static Model_mp_lit **MP2** (modelType, random_field)
- static Model_mp_lit **MP2** (modelType, simulation)
- static Model_mp_lit **MP2** (modelType, surrogate)
- static Model_mp_lit **MP2** (surrogateType, hierarchical)
- static Model_mp_lit **MP2** (surrogateType, non_hierarchical)
- static Model_mp_lit **MP2** (surrogateType, global_exp_gauss_proc)
- static Model_mp_lit **MP2** (surrogateType, global_exp_poly)

- static Model_mp_lit **MP2** (surrogateType, global_function_train)
- static Model_mp_lit **MP2** (surrogateType, global_gaussian)
- static Model_mp_lit **MP2** (surrogateType, global_kriging)
- static Model_mp_lit **MP2** (surrogateType, global_mars)
- static Model_mp_lit **MP2** (surrogateType, global_moving_least_squares)
- static Model_mp_lit **MP2** (surrogateType, global_neural_network)
- static Model_mp_lit **MP2** (surrogateType, global_polynomial)
- static Model_mp_lit **MP2** (surrogateType, global_radial_basis)
- static Model_mp_lit **MP2** (surrogateType, global_voronoi_surrogate)
- static Model_mp_lit **MP2** (surrogateType, local_taylor)
- static Model_mp_lit **MP2** (surrogateType, multipoint_qmea)
- static Model_mp_lit **MP2** (surrogateType, multipoint_tana)
- static Model_mp_lit **MP2** (trendOrder, none)
- static Model_mp_lit **MP2** (trendOrder, constant)
- static Model_mp_lit **MP2** (trendOrder, linear)
- static Model_mp_lit **MP2** (trendOrder, reduced_quadratic)
- static Model_mp_lit **MP2** (trendOrder, quadratic)
- static Model_mp_ord **MP2s** (approxCorrectionOrder, 0)
- static Model_mp_ord **MP2s** (approxCorrectionOrder, 1)
- static Model_mp_ord **MP2s** (approxCorrectionOrder, 2)
- static Model_mp_ord **MP2s** (polynomialOrder, 1)
- static Model_mp_ord **MP2s** (polynomialOrder, 2)
- static Model_mp_ord **MP2s** (polynomialOrder, 3)
- static Model_mp_type **MP2s** (approxCorrectionType, ADDITIVE_CORRECTION)
- static Model_mp_type **MP2s** (approxCorrectionType, COMBINED_CORRECTION)
- static Model_mp_type **MP2s** (approxCorrectionType, MULTIPLICATIVE_CORRECTION)
- static Model_mp_type **MP2s** (pointsManagement, MINIMUM_POINTS)
- static Model_mp_type **MP2s** (pointsManagement, RECOMMENDED_POINTS)
- static Model_mp_type **MP2s** (subMethodScheduling, MASTER_SCHEDULING)
- static Model_mp_type **MP2s** (method_rotation, ROTATION_METHOD_UNRANKED)
- static Model_mp_type **MP2s** (method_rotation, ROTATION_METHOD_RANKED)
- static Model_mp_type **MP2s** (subMethodScheduling, PEER_SCHEDULING)
- static Model_mp_utype **MP2s** (analyticCovIdForm, EXP_L2)
- static Model_mp_utype **MP2s** (analyticCovIdForm, EXP_L1)
- static Model_mp_utype **MP2s** (exportApproxVarianceFormat, TABULAR_NONE)
- static Model_mp_utype **MP2s** (exportApproxVarianceFormat, TABULAR_HEADER)
- static Model_mp_utype **MP2s** (exportApproxVarianceFormat, TABULAR_EVAL_ID)
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- static Model_mp_utype **MP2s** (exportApproxVarianceFormat, TABULAR_ANNOTATED)
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- static Model_mp_utype **MP2s** (importChallengeFormat, TABULAR_IFACE_ID)
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- static Model_mp_utype **MP2s** (modelExportFormat, ALGEBRAIC_CONSOLE)
- static Model_mp_utype **MP2s** (modelImportFormat, TEXT_ARCHIVE)
- static Model_mp_utype **MP2s** (modelImportFormat, BINARY_ARCHIVE)
- static Model_mp_utype **MP2s** (randomFieldIdForm, RF_KARHUNEN_LOEVE)
- static Model_mp_utype **MP2s** (randomFieldIdForm, RF_PCA_GP)
- static Model_mp_utype **MP2s** (subspaceNormalization, SUBSPACE_NORM_MEAN_VALUE)
- static Model_mp_utype **MP2s** (subspaceNormalization, SUBSPACE_NORM_MEAN_GRAD)
- static Model_mp_utype **MP2s** (subspaceNormalization, SUBSPACE_NORM_LOCAL_GRAD)
- static Model_mp_utype **MP2s** (subspaceSampleType, SUBMETHOD_LHS)
- static Model_mp_utype **MP2s** (subspaceSampleType, SUBMETHOD_RANDOM)

- static Model_mp_utype **MP2s** (subspaceIdCVMethod, MINIMUM_METRIC)
- static Model_mp_utype **MP2s** (subspaceIdCVMethod, RELATIVE_TOLERANCE)
- static Model_mp_utype **MP2s** (subspaceIdCVMethod, DECREASE_TOLERANCE)
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- static Real **MP_** (decreaseTolerance)
- static Real **MP_** (discontGradThresh)
- static Real **MP_** (discontJumpThresh)
- static Real **MP_** (krigingNugget)
- static Real **MP_** (percentFold)
- static Real **MP_** (relTolerance)
- static Real **MP_** (truncationTolerance)
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- static bool **MP_** (subspaceIdCV)

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- static IntSet **MP_** (idQuasiHessians)
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- static RealVector **MP_** (simVariance)
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- static RealVector **MP_** (fdHessStepSize)
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- static RealVector **MP_** (nonlinearIneqScales)
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- static Resp_mp_lit **MP2** (gradientType, mixed)
- static Resp_mp_lit **MP2** (gradientType, none)
- static Resp_mp_lit **MP2** (gradientType, numerical)
- static Resp_mp_lit **MP2** (hessianType, analytic)
- static Resp_mp_lit **MP2** (hessianType, mixed)
- static Resp_mp_lit **MP2** (hessianType, none)
- static Resp_mp_lit **MP2** (hessianType, numerical)
- static Resp_mp_lit **MP2** (hessianType, quasi)
- static Resp_mp_lit **MP2** (intervalType, central)

- static Resp_mp_lit **MP2** (intervalType, forward)
- static Resp_mp_lit **MP2** (methodSource, dakota)
- static Resp_mp_lit **MP2** (methodSource, vendor)
- static Resp_mp_lit **MP2** (fdGradStepType, absolute)
- static Resp_mp_lit **MP2** (fdGradStepType, bounds)
- static Resp_mp_lit **MP2** (fdGradStepType, relative)
- static Resp_mp_lit **MP2** (fdHessStepType, absolute)
- static Resp_mp_lit **MP2** (fdHessStepType, bounds)
- static Resp_mp_lit **MP2** (fdHessStepType, relative)
- static Resp_mp_lit **MP2** (quasiHessianType, bfgs)
- static Resp_mp_lit **MP2** (quasiHessianType, damped_bfgs)
- static Resp_mp_lit **MP2** (quasiHessianType, sr1)
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- static String **MP_** (scalarDataFileName)
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- static StringArray **MP_** (nonlinearIneqScaleTypes)
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- static StringArray **MP_** (primaryRespFnSense)
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- static bool **MP_** (centralHess)
- static bool **MP_** (interpolateFlag)
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- static bool **MP_** (readFieldCoords)
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- static size_t **MP_** (numScalarObjectiveFunctions)
- static size_t **MP_** (numScalarResponseFunctions)
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- static Resp_mp_utype **MP2s** (scalarDataFormat, TABULAR_EVAL_ID)
- static Resp_mp_utype **MP2s** (scalarDataFormat, TABULAR_EXPER_ANNOT)
- static Env_mp_utype **MP2s** (postRunInputFormat, TABULAR_NONE)
- static Env_mp_utype **MP2s** (postRunInputFormat, TABULAR_HEADER)
- static Env_mp_utype **MP2s** (postRunInputFormat, TABULAR_EVAL_ID)
- static Env_mp_utype **MP2s** (postRunInputFormat, TABULAR_IFACE_ID)
- static Env_mp_utype **MP2s** (postRunInputFormat, TABULAR_ANNOTATED)
- static Env_mp_utype **MP2s** (preRunOutputFormat, TABULAR_NONE)
- static Env_mp_utype **MP2s** (preRunOutputFormat, TABULAR_HEADER)
- static Env_mp_utype **MP2s** (preRunOutputFormat, TABULAR_EVAL_ID)
- static Env_mp_utype **MP2s** (preRunOutputFormat, TABULAR_IFACE_ID)
- static Env_mp_utype **MP2s** (preRunOutputFormat, TABULAR_ANNOTATED)
- static Env_mp_utype **MP2s** (tabularFormat, TABULAR_NONE)

- static Env_mp_utype **MP2s** (tabularFormat, TABULAR_HEADER)
- static Env_mp_utype **MP2s** (tabularFormat, TABULAR_EVAL_ID)
- static Env_mp_utype **MP2s** (tabularFormat, TABULAR_IFACE_ID)
- static Env_mp_utype **MP2s** (tabularFormat, TABULAR_ANNOTATED)
- static Env_mp_utype **MP2s** (resultsOutputFormat, RESULTS_OUTPUT_TEXT)
- static Env_mp_utype **MP2s** (resultsOutputFormat, RESULTS_OUTPUT_HDF5)
- static Env_mp_utype **MP2s** (modelEvalsSelection, MODEL_EVAL_STORE_TOP_METHOD)
- static Env_mp_utype **MP2s** (modelEvalsSelection, MODEL_EVAL_STORE_NONE)
- static Env_mp_utype **MP2s** (modelEvalsSelection, MODEL_EVAL_STORE_ALL)
- static Env_mp_utype **MP2s** (modelEvalsSelection, MODEL_EVAL_STORE_ALL_METHODS)
- static Env_mp_utype **MP2s** (interfEvalsSelection, INTERF_EVAL_STORE_SIMULATION)
- static Env_mp_utype **MP2s** (interfEvalsSelection, INTERF_EVAL_STORE_NONE)
- static Env_mp_utype **MP2s** (interfEvalsSelection, INTERF_EVAL_STORE_ALL)
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- static String **MP_** (outputFile)
- static String **MP_** (postRunInput)
- static String **MP_** (postRunOutput)
- static String **MP_** (preRunInput)
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- static bool **MP_** (tabularDataFlag)
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- static int **MP_** (stopRestart)
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- static size_t **MP_** (numContinuousStateVars)
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- static size_t **MP_** (numLognormalUncVars)
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- static IntVector **VP_** (DIlb)
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- static IntVector **MP_** (discreteStateRangeVars)
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- static IntVector **VP_** (DIub)
- static IntVector **MP_** (histogramPointIntUncVars)
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- static IntVector **VP_** (ddsia)
- static IntVector **VP_** (ddssa)
- static IntVector **VP_** (ddsra)
- static IntVector **VP_** (dusi)
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- static IntArray **VP_** (nddss)
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- static RealVector **VP_** (CIlb)
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- static RealVector **VP_** (DSRp)
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- static StringArray **MP_** (continuousStateLabels)

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- static StringArray **MP_** (discreteUncSetStrVars)
- static StringArray **MP_** (discreteStateSetStrVars)
- static StringArray **MP_** (histogramPointStrUncVars)
- static StringArray **MP_** (linearEqScaleTypes)
- static StringArray **MP_** (linearIneqScaleTypes)
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- static StringArray **VP_** (ddss)
- static StringArray **VP_** (duss)
- static StringArray **VP_** (dsss)
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- static BitArray **MP_** (discreteDesignSetRealCat)
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- static BitArray **MP_** (discreteUncSetIntCat)
- static BitArray **MP_** (discreteUncSetRealCat)
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- static Var_brv **MP2s** (betaUncBetas, 0.)
- static Var_brv **MP2s** (exponentialUncBetas, 0.)
- static Var_brv **MP2s** (exponentialUncVars, 0.)
- static Var_brv **MP2s** (frechetUncAlphas, 2.)
- static Var_brv **MP2s** (gammaUncAlphas, 0.)
- static Var_brv **MP2s** (gammaUncBetas, 0.)
- static Var_brv **MP2s** (gammaUncVars, 0.)
- static Var_brv **MP2s** (gumbelUncAlphas, 0.)
- static Var_brv **MP2s** (lognormalUncErrFacts, 1.)
- static Var_brv **MP2s** (lognormalUncLambdas, 0.)
- static Var_brv **MP2s** (lognormalUncLowerBnds, 0.)
- static Var_brv **MP2s** (lognormalUncMeans, 0.)
- static Var_brv **MP2s** (lognormalUncStdDevs, 0.)
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- static Var_brv **MP2s** (lognormalUncZetas, 0.)
- static Var_brv **MP2s** (loguniformUncLowerBnds, 0.)
- static Var_brv **MP2s** (loguniformUncUpperBnds, std::numeric_limits< Real >::infinity())
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- static Var_brv **MP2s** (poissonUncLambdas, 0.)
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- static Var_brv **MP2s** (triangularUncUpperBnds, std::numeric_limits< Real >::infinity())
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- static Var_brv **MP2s** (uniformUncUpperBnds, std::numeric_limits< Real >::infinity())
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- static Var_brv **MP2s** (weibullUncBetas, 0.)
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- static Var_biv **MP2s** (binomialUncVars, 0)
- static Var_biv **MP2s** (geometricUncVars, 0)

- static Var_biv **MP2s** (hyperGeomUncNumDrawn, 0)
- static Var_biv **MP2s** (hyperGeomUncSelectedPop, 0)
- static Var_biv **MP2s** (hyperGeomUncTotalPop, 0)
- static Var_biv **MP2s** (hyperGeomUncVars, 0)
- static Var_biv **MP2s** (negBinomialUncNumTrials, 0)
- static Var_biv **MP2s** (negBinomialUncVars, 0)
- static Var_biv **MP2s** (poissonUncVars, 0)
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- static Var_mp_type **Vtype** (varsDomain, RELAXED_DOMAIN)
- static Var_mp_type **Vtype** (varsView, ALL_VIEW)
- static Var_mp_type **Vtype** (varsView, DESIGN_VIEW)
- static Var_mp_type **Vtype** (varsView, UNCERTAIN_VIEW)
- static Var_mp_type **Vtype** (varsView, ALEATORY_UNCERTAIN_VIEW)
- static Var_mp_type **Vtype** (varsView, EPISTEMIC_UNCERTAIN_VIEW)
- static Var_mp_type **Vtype** (varsView, STATE_VIEW)
- template< class ContainerT >
  void flatten_num_array (const std::vector< ContainerT > &input_array, IntArray ∗∗pia)

  Free convenience function that flatten sizes of an array of std containers; takes an array of containers and returns an IntArray containing the sizes of each container in the input array. Note: Did not specialize for vector<RealVector> as no current use cases.
- void **dn2f_** (int ∗n, int ∗p, Real ∗x, Calcrj, int ∗iv, int ∗liv, int ∗lv, Real ∗v, int ∗ui, void ∗ur, Vf)
- void **dn2fb_** (int ∗n, int ∗p, Real ∗x, Real ∗b, Calcrj, int ∗iv, int ∗liv, int ∗lv, Real ∗v, int ∗ui, void ∗ur, Vf)
- void **dn2g_** (int ∗n, int ∗p, Real ∗x, Calcrj, Calcrj, int ∗iv, int ∗liv, int ∗lv, Real ∗v, int ∗ui, void ∗ur, Vf)
- void **dn2gb_** (int ∗n, int ∗p, Real ∗x, Real ∗b, Calcrj, Calcrj, int ∗iv, int ∗liv, int ∗lv, Real ∗v, int ∗ui, void ∗ur, Vf)
- void **divset_** (int ∗, int ∗, int ∗, int ∗, Real ∗)
- double **dr7mdc_** (int ∗)
- static void **Rswapchk** (Nl2Misc ∗q)
- static int **hasnaninf** (const double ∗d, int n)
- NLPQLPOptimizer ∗ **new_NLPQLPOptimizer** (ProblemDescDB &problem_db, Model &model)
- NLPQLPOptimizer ∗ **new_NLPQLPOptimizer** (Model &model)
- void **print_c3_sobol_indices** (double value, size_t ninteract, size_t ∗interactions, void ∗arg)
- static const RealVector ∗ **static_lev_cost_vec** (NULL)
- static size_t ∗ **static_qoi** (NULL)
- static const Real ∗ **static_eps_sq_div_2** (NULL)
- static const RealVector ∗ **static_Nlq_pilot** (NULL)
- static const size_t ∗ **static_numFunctions** (NULL)
- static const size_t ∗ **static_qoiAggregation** (NULL)
- static int ∗ **static_randomSeed** (NULL)
- static const IntRealMatrixMap ∗ **static_sum_Ql** (NULL)
- static const IntRealMatrixMap ∗ **static_sum_Qlm1** (NULL)
- static const
  IntIntPairRealMatrixMap ∗ **static_sum_QlQlm1** (NULL)
- static const RealMatrix ∗ **static_scalarization_response_mapping** (NULL)
- static const IntRealMatrixMap ∗ **static_levQoisamplesmatrixMap** (NULL)
- static const short ∗ **static_cov_approximation_type** (NULL)
- static const Real ∗ **static_mu_four_L** (NULL)
- static const Real ∗ **static_mu_four_H** (NULL)
- static const Real ∗ **static_var_L** (NULL)
- static const Real ∗ **static_var_H** (NULL)
- static const Real ∗ **static_Ax** (NULL)
- NOWPACOptimizer ∗ **new_NOWPACOptimizer** (ProblemDescDB &problem_db, Model &model)
- NOWPACOptimizer ∗ **new_NOWPACOptimizer** (Model &model)
- NPSOLOptimizer ∗ **new_NPSOLOptimizer** (ProblemDescDB &problem_db)
- NPSOLOptimizer ∗ **new_NPSOLOptimizer1** (Model &model)
- NPSOLOptimizer ∗ **new_NPSOLOptimizer2** (Model &model, int derivative_level, Real conv_tol)

- NPSOLOptimizer ∗ **new_NPSOLOptimizer3** (const RealVector &initial_point, const RealVector &var_lower_bnds, const RealVector &var_upper_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_lower_bnds, const RealVector &lin_ineq_upper_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_targets, const RealVector &nonlin_ineq_lower_bnds, const RealVector &nonlin_ineq_upper_bnds, const RealVector &nonlin_eq_targets, void(∗user_obj_eval)(int &, int &, double ∗, double &, double ∗, int &), void(∗user_con_eval)(int &, int &, int &, int &, int ∗, double ∗, double ∗, double ∗, int &), int derivative_level, Real conv_tol)
- NPSOLOptimizer ∗ **new_NPSOLOptimizer** (ProblemDescDB &problem_db, Model &model)
- NPSOLOptimizer ∗ **new_NPSOLOptimizer** (Model &model)
- NPSOLOptimizer ∗ **new_NPSOLOptimizer** (Model &model, int, Real)
- NPSOLOptimizer ∗ **new_NPSOLOptimizer** (const RealVector &initial_point, const RealVector &var_lower_bnds, const RealVector &var_upper_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_lower_bnds, const RealVector &lin_ineq_upper_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_targets, const RealVector &nonlin_ineq_lower_bnds, const RealVector &nonlin_ineq_upper_bnds, const RealVector &nonlin_eq_targets, void(∗user_obj_eval)(int &, int &, double ∗, double &, double ∗, int &), void(∗user_con_eval)(int &, int &, int &, int &, int ∗, double ∗, double ∗, double ∗, int &), int derivative_level, Real conv_tol)
- void start_dakota_heartbeat (int)
- void **dak_sigcatch** (int sig)
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, ParallelLevel &pl)

  MPIUnpackBuffer extraction operator for ParallelLevel. Calls read(MPIUnpackBuffer&).
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const ParallelLevel &pl)

  MPIPackBuffer insertion operator for ParallelLevel. Calls write(MPIPackBuffer&).
- std::istream & operator>> (std::istream &s, ParamResponsePair &pair)

  std::istream extraction operator for ParamResponsePair
- std::ostream & operator<< (std::ostream &s, const ParamResponsePair &pair)

  std::ostream insertion operator for ParamResponsePair
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, ParamResponsePair &pair)

  MPIUnpackBuffer extraction operator for ParamResponsePair.
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const ParamResponsePair &pair)

  MPIPackBuffer insertion operator for ParamResponsePair.
- bool operator== (const ParamResponsePair &pair1, const ParamResponsePair &pair2)

  equality operator for ParamResponsePair
- bool operator!= (const ParamResponsePair &pair1, const ParamResponsePair &pair2)

  inequality operator for ParamResponsePair
- void **copy_gradient** (int const fun_idx, std::vector< std::vector< double >> const &source, RealMatrix &dest)
- void **copy_hessian** (std::vector< std::vector< double >> const &source, RealSymMatrix &dest)
- static void **Bad_name** (const String &entry_name, const String &where)
- static void **Locked_db** ()
- static void **Null_rep** (const String &who)
- std::pair< std::string,
  std::string > **split_entry_name** (const std::string &entry_name, const std::string &context_msg)
- boost::regex **PARAMS_TOKEN** ("\\{PARAMETERS\\}")
- boost::regex **RESULTS_TOKEN** ("\\{RESULTS\\}")
- String substitute_params_and_results (const String &driver, const String &params, const String &results)

  Substitute parameters and results file names into driver strings.
- MPIUnpackBuffer & operator>> (MPIUnpackBuffer &s, ProgramOptions &p_opt)

  MPIUnpackBuffer extraction operator.
- MPIPackBuffer & operator<< (MPIPackBuffer &s, const ProgramOptions &p_opt)

  MPIPackBuffer insertion operator.
- bool set_compare (const ParamResponsePair &database_pr, const ActiveSet &search_set)

  search function for a particular ParamResponsePair within a PRPList based on ActiveSet content (request vector and derivative variables vector)

- bool id_vars_exact_compare (const ParamResponsePair &database_pr, const ParamResponsePair &search-_pr)

  search function for a particular ParamResponsePair within a PRPMultiIndex
- std::size_t hash_value (const ParamResponsePair &prp)

  hash_value for ParamResponsePairs stored in a PRPMultiIndex
- PRPCacheHIter hashedCacheBegin (PRPCache &prp_cache)

  hashed definition of cache begin
- PRPCacheHIter hashedCacheEnd (PRPCache &prp_cache)

  hashed definition of cache end
- PRPQueueHIter hashedQueueBegin (PRPQueue &prp_queue)

  hashed definition of queue begin
- PRPQueueHIter hashedQueueEnd (PRPQueue &prp_queue)

  hashed definition of queue end
- PRPCacheHIter lookup_by_val (PRPMultiIndexCache &prp_cache, const ParamResponsePair &search_pr)

  find a ParamResponsePair based on the interface id, variables, and ActiveSet search data within search_pr.
- PRPCacheHIter lookup_by_val (PRPMultiIndexCache &prp_cache, const String &search_interface_id, const Variables &search_vars, const ActiveSet &search_set)

  find a ParamResponsePair within a PRPMultiIndexCache based on the interface id, variables, and ActiveSet search data
- PRPCacheOIter **lookup_by_nearby_val** (PRPMultiIndexCache &prp_cache, const String &search_-interface_id, const Variables &search_vars, const ActiveSet &search_set, Real tol)
- PRPCacheOIter lookup_by_ids (PRPMultiIndexCache &prp_cache, const IntStringPair &search_ids)

  find a ParamResponsePair within a PRPMultiIndexCache based on search_ids (i.e. std::pair<eval_id,interface_id>) search data
- PRPCacheOIter **lookup_by_ids** (PRPMultiIndexCache &prp_cache, const IntStringPair &search_ids, const ParamResponsePair &search_pr)
- PRPQueueHIter lookup_by_val (PRPMultiIndexQueue &prp_queue, const ParamResponsePair &search_pr)

  find a ParamResponsePair based on the interface id, variables, and ActiveSet search data within search_pr.
- PRPQueueHIter lookup_by_val (PRPMultiIndexQueue &prp_queue, const String &search_interface_id, const Variables &search_vars, const ActiveSet &search_set)

  find a ParamResponsePair within a PRPMultiIndexQueue based on interface id, variables, and ActiveSet search data
- PRPQueueOIter lookup_by_eval_id (PRPMultiIndexQueue &prp_queue, int search_id)

  find a ParamResponsePair within a PRPMultiIndexQueue based on search_id (i.e. integer eval_id) search data
- void print_usage (std::ostream &s)

  print restart utility help message
- void print_restart (StringArray pos_args, String print_dest)

  print a restart file
- void print_restart_pdb (StringArray pos_args, String print_dest)

  print a restart file (PDB format)
- void print_restart_tabular (StringArray pos_args, String print_dest, unsigned short tabular_format, int tabular-_precision)

  print a restart file (tabular format)
- void read_neutral (StringArray pos_args)

  read a restart file (neutral file format)
- void repair_restart (StringArray pos_args, String identifier_type)

  repair a restart file by removing corrupted evaluations
- void concatenate_restart (StringArray pos_args)

  concatenate multiple restart files
- String method_results_hdf5_link_name (const StrStrSizet &iterator_id)

  Create a method results name (HDF5 link name) from iterator_id.
- String method_hdf5_link_name (const StrStrSizet &iterator_id)

  Create a method name (HDF5 link name) from iterator_id.

- String execution_hdf5_link_name (const StrStrSizet &iterator_id)

    Create an execution name (HDF5 link name) from iterator_id.
- String **object_hdf5_link_name** (const StrStrSizet &iterator_id, const StringArray &location)
- template<typename ScaleType >
  String scale_hdf5_link_name (const StrStrSizet &iterator_id, const StringArray &location, const ScaleType &scale)

    Create a scale name (hdf5 link name) for a scale from an iterator_id, the name of the result, the name of the response (can be empty), and the scale itself.
- template<typename T >
  void expand_for_fields_sdv (const SharedResponseData &srd, const T &src_array, const String &src_desc, bool allow_by_element, T &expanded_array)

    expand primary response specs in SerialDenseVectors, e.g. scales, for fields no change on empty, expands 1 and num_groups, copies num_elements
- template<typename T >
  void expand_for_fields_stl (const SharedResponseData &srd, const T &src_array, const String &src_desc, bool allow_by_element, T &expanded_array)

    expand primary response specs in STL containers, e.g. scale types, for fields no change on empty, expands 1 and num_groups, copies num_elements
- static HANDLE ∗ **wait_setup** (std::map< pid_t, int > ∗M, size_t ∗pn)
- static int **wait_for_one** (size_t n, HANDLE ∗h, int req1, size_t ∗pi)
- void **gauss_legendre_pts_wts_1D** (int level, RealVector &result_0, RealVector &result_1)
- void **lagrange_interpolation_1d** (const RealVector &samples, const RealVector &abscissa, const RealVector &values, RealVector &result)
- void **kronecker_product_2d** (const RealMatrix &matrix1, const RealMatrix &matrix2, RealMatrix &matrix)
- void **get_chebyshev_points** (int order, RealVector &points)
- void **chebyshev_derivative_matrix** (int order, RealMatrix &derivative_matrix, RealVector &points)
- int salinas_main (int argc, char ∗argv[], MPI_Comm ∗comm)

    subroutine interface to SALINAS simulation code
- std::string **get_cwd_str** ()
- std::vector< std::string > get_pathext ()
- bool contains (const bfs::path &dir_path, const std::string &file_name, boost::filesystem::path &complete_filepath)

Variables

- PRPCache data_pairs

    contains all parameter/response pairs.
- double PI = boost::math::constants::pi<double>()

    constant pi
- double HALF_LOG_2PI = std::log(2.0∗PI)/2.0

    constant log(2∗pi)/2.0
- short abort_mode = ABORT_EXITS

    by default Dakota exits or calls MPI_Abort on errors
- std::ostream ∗ dakota_cout = &std::cout

    `DAKOTA stdout initially points to`
    < std::cout, but may be redirected to a tagged ofstream if there are < concurrent iterators.
- std::ostream ∗ dakota_cerr = &std::cerr

    `DAKOTA stderr initially points to`
    < std::cerr, but may be redirected to a tagged ofstream if there are < concurrent iterators.
- ResultsManager iterator_results_db

    Global results database for iterator results.
- EvaluationStore evaluation_store_db

    Global database for evaluation storage.

- int write_precision = 10

  used in ostream data output functions < (restart_util.cpp overrides default value)
- MPIManager dummy_mpi_mgr

  dummy MPIManager for ref initialization
- ProgramOptions dummy_prg_opt

  dummy ProgramOptions for ref initialization
- OutputManager dummy_out_mgr

  dummy OutputManager for ref initialization
- ParallelLibrary dummy_lib

  dummy ParallelLibrary for ref initialization
- ProblemDescDB dummy_db

  dummy ProblemDescDB for ref initialization
- int mc_ptr_int = 0

  global pointer for ModelCenter API
- int dc_ptr_int = 0

  global pointer for ModelCenter eval DB
- ProblemDescDB ∗ Dak_pddb

  set by ProblemDescDB, for use in parsing
- const size_t SZ_MAX = std::numeric_limits<size_t>::max()

  special value returned by index() when entry not found
- const size_t **_NPOS** = SZ_MAX
- const double BIG_REAL_BOUND = 1.0e+30

  bound beyond which constraints are considered inactive
- static UShortStrBimap method_map

  bimap between method enums and strings; only used in this compilation unit
- static UShortStrBimap submethod_map

  bimap between sub-method enums and strings; only used in this compilation unit (using bimap for consistency, though at time of addition, only uni-directional mapping is supported)
- Interface dummy_interface

  ```
  dummy Interface object used for mandatory
  ```
  < reference initialization or default virtual < function return by reference when a real < Interface instance is unavailable
- Model dummy_model

  ```
  dummy Model object used for mandatory reference
  ```
  < initialization or default virtual function < return by reference when a real Model instance < is unavailable
- Iterator dummy_iterator

  ```
  dummy Iterator object used for mandatory
  ```
  < reference initialization or default virtual < function return by reference when a real < Iterator instance is unavailable
- Dakota_funcs ∗ **DF**
- Dakota_funcs **DakFuncs0**
- const Real **REAL_DSET_FILL_VAL** = NAN
- const int **INT_DSET_FILL_VAL** = INT_MAX
- const String **STR_DSET_FILL_VAL** = ""
- const int **HDF5_CHUNK_SIZE** = 40000
- const char ∗ FIELD_NAMES []
- const int NUMBER_OF_FIELDS = 23
- static const int **MPI_COMM_WORLD** = 1
- static const int **MPI_COMM_NULL** = 0
- static const int **MPI_COMM_SELF** = 92
- static const int **MPI_ANY_TAG** = -1
- static void ∗ **MPI_REQUEST_NULL** = NULL
- FILE ∗ **nidrin**
- const size_t NIDR_MAX_ERROR_LEN = 8192

maximum error length is roughly 100 lines at 80 char; using fixed error length instead of investing in converting to vsnprintf (C++11)

- static const char ∗ **auto_log_scaletypes** [ ] = { "auto", "log", "none", 0 }
- static Var_uinfo **CAUVLbl** [CAUVar_Nkinds]
- static Var_uinfo **DAUIVLbl** [DAUIVar_Nkinds]
- static Var_uinfo **DAUSVLbl** [DAUSVar_Nkinds]
- static Var_uinfo **DAURVLbl** [DAURVar_Nkinds]
- static Var_uinfo **CEUVLbl** [CEUVar_Nkinds]
- static Var_uinfo **DEUIVLbl** [DEUIVar_Nkinds]
- static Var_uinfo **DEUSVLbl** [DEUSVar_Nkinds]
- static Var_uinfo **DEURVLbl** [DEURVar_Nkinds]
- static Var_uinfo **DiscSetLbl** [DiscSetVar_Nkinds]
- static VarLabelChk DesignAndStateLabelsCheck [ ]

  Variables label array designations for design and state. All non-uncertain variables need to be in this array. Used in check_variables_node to check lengths and make_variable_defaults to build labels.

- static VLreal VLUncertainReal [NUM_UNC_REAL_CONT]

  Variables labels/bounds/values check array for real-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., CAUVLbl, with the contiguous container in which they are stored.

- static VLint VLUncertainInt [NUM_UNC_INT_CONT]

  Variables labels/bounds/values check array for integer-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., DAUIVLbl, with the contiguous container in which they are stored.

- static VLstr VLUncertainStr [NUM_UNC_STR_CONT]

  Variables labels/bounds/values check array for string-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., DAUSVLbl, with the contiguous container in which they are stored.

- static int VLR_aleatory [NUM_UNC_REAL_CONT] = { 1, 0, 1, 0 }

  which uncertain real check array containers are aleatory (true = 1)

- static int VLI_aleatory [NUM_UNC_INT_CONT] = { 1, 0 }

  which uncertain integer check array containers are aleatory (true = 1)

- static int VLS_aleatory [NUM_UNC_STR_CONT] = { 1, 0 }

  which uncertain string check array containers are aleatory (true = 1)

- static Var_check **var_mp_check_cv** [ ]
- static Var_check **var_mp_check_dset** [ ]
- static Var_check **var_mp_check_cau** [ ]
- static Var_check **var_mp_check_daui** [ ]
- static Var_check **var_mp_check_daus** [ ]
- static Var_check **var_mp_check_daur** [ ]
- static Var_check **var_mp_check_ceu** [ ]
- static Var_check **var_mp_check_deui** [ ]
- static Var_check **var_mp_check_deus** [ ]
- static Var_check **var_mp_check_deur** [ ]
- static Var_rcheck var_mp_cbound [ ]

  This is used within check_variables_node(): Var_RealBoundIPCheck() is applied to validate bounds and initial points.

- static Var_icheck var_mp_drange [ ]

  This is used in check_variables_node(): Var_IntBoundIPCheck() is applied to validate bounds and initial points, and in make_variable_defaults(): Vgen_∗ is called to infer bounds.

- TKFactoryDIPC tk_factory_dipc ("dakota_dipc_tk")

  Static registration of RW TK with the QUESO TK factory.

- TKFactoryDIPCLogit tk_factory_dipclogit ("dakota_dipc_logit_tk")

  Static registration of Logit RW TK with the QUESO TK factory.

- static time_t **start_time**
- const double SCALING_MIN_SCALE = 1.0e10∗DBL_MIN

minimum value allowed for a characteristic value when scaling; ten orders of magnitude greater than DBL_MIN

- const double SCALING_MIN_LOG = SCALING_MIN_SCALE

  lower bound on domain of logarithm function when scaling
- const double SCALING_LOGBASE = 10.0

  logarithm base to be used when scaling
- const double SCALING_LN_LOGBASE = std::log(SCALING_LOGBASE)

  ln(SCALING_LOGBASE); needed in transforming variables in several places
- const char ∗ SCI_FIELD_NAMES [ ]
- const int SCI_NUMBER_OF_FIELDS = 26
- const int LARGE_SCALE = 100

  a (perhaps arbitrary) definition of large scale; choose a large-scale algorithm if numVars >= LARGE_SCALE
- const double POW_VAL = 1.0

  offset used text_book exponent: 1.0 is nominal, 1.4 used for B&B testing
- const String LEV_REF = "Dakota"

  levenshtein_distance computes the distance between its argument and this

13.2.1 Detailed Description

The primary namespace for DAKOTA. The Dakota namespace encapsulates the core classes of the DAKOTA framework and prevents name clashes with third-party libraries from methods and packages. The C++ source files defining these core classes reside in Dakota/src as ∗.[ch]pp.

13.2.2 Typedef Documentation

13.2.2.1 typedef bmi::multi_index_container<**Dakota::ParamResponsePair**, bmi::indexed_by< bmi::ordered_non_-unique<bmi::tag<ordered>, bmi::const_mem_fun<**Dakota::ParamResponsePair**, const IntStringPair&, **&Dakota::ParamResponsePair::eval_interface_ids**> >, bmi::hashed_non_unique<bmi::tag<hashed>, bmi::identity<**Dakota::ParamResponsePair**>, **partial_prp_hash**, **partial_prp_equality**> > > **PRPMultiIndexCache**

Boost Multi-Index Container for globally caching ParamResponsePairs.

For a global cache, both evaluation and interface id's are used for tagging ParamResponsePair records.

13.2.2.2 typedef bmi::multi_index_container<**Dakota::ParamResponsePair**, bmi::indexed_by< bmi::ordered_unique<bmi::tag<ordered>, bmi::const_mem_fun<**Dakota::ParamResponsePair**, int, **&Dakota::ParamResponsePair::eval_id**> >, bmi::hashed_non_unique<bmi::tag<hashed>, bmi::identity<**Dakota::ParamResponsePair**>, **partial_prp_hash**, **partial_prp_equality**> > > **PRPMultiIndexQueue**

Boost Multi-Index Container for locally queueing ParamResponsePairs.

For a local queue, interface id's are expected to be consistent, such that evaluation id's are sufficient for tracking particular evaluations.

13.2.3 Enumeration Type Documentation

13.2.3.1 anonymous enum

Sub-methods, including sampling, inference algorithm, opt algorithm types.

Enumerator

SUBMETHOD_COLLABORATIVE Type of hybrid meta-iterator:

13.2.4 Function Documentation

13.2.4.1 CommandShell & flush (CommandShell & *shell*)

convenient shell manipulator function to "flush" the shell

global convenience function for manipulating the shell; invokes the class member flush function.

References CommandShell::flush().

Referenced by HDF5IOHelper::append_empty(), HDF5IOHelper::create_dataset(), HDF5IOHelper::create_empty-_dataset(), HDF5IOHelper::create_group(), SysCallApplicInterface::spawn_analysis_to_shell(), SysCallApplic-Interface::spawn_evaluation_to_shell(), SysCallApplicInterface::spawn_input_filter_to_shell(), and SysCallApplic-Interface::spawn_output_filter_to_shell().

13.2.4.2 void Dakota::apply_matrix_partial (const MatrixType & *M,* const VectorType & *v1,* VectorType & *v2*)

Applies a RealMatrix to a vector (or subset of vector) v1.

Optionally works with a subset of the passed vectors; applies the matrix M to the first M.numCols() entries in v1, and populates the first M.numRows entries in v2.

References abort_handler().

Referenced by apply_linear_constraints(), DakotaROLIneqConstraintsHess::applyAdjointHessian(), DakotaRO-LEqConstraintsHess::applyAdjointHessian(), DakotaROLIneqConstraintsGrad::applyJacobian(), DakotaROLEq-ConstraintsGrad::applyJacobian(), and DakotaROLObjectiveHess::hessVec().

13.2.4.3 void Dakota::apply_matrix_transpose_partial (const RealMatrix & *M,* const VectorType & *v1,* VectorType & *v2*)

Applies transpose of a RealMatrix to a vector (or subset of vector) v1.

Optionally works with a subset of the passed vectors; applies the matrix M^T to the first M.numRows() entries in v1, and populates the first M.numCols() entries in v2.

References abort_handler().

Referenced by DakotaROLIneqConstraintsGrad::applyAdjointJacobian(), and DakotaROLEqConstraintsGrad-::applyAdjointJacobian().

13.2.4.4 void abort_throw_or_exit (int *dakota_code*)

throw or exit depending on abort_mode

Throw a system_error or call std::exit, with (256 + dakota_code), where dakota_code $<$ 0

RATIONALE: Avoid common "standard" exit codes and signals (signum.h) as well as uncaught signals / uncatchable SIGKILL which return 128

- <signum> on Linux = [129, 192]

Return a value in [0,255] since some operating systems only return the 8 least significant bits, leaves [193, 255] for Dakota. This should make return codes consistent cross-platform.

References abort_mode.

Referenced by abort_handler(), and ParallelLibrary::abort_helper().

13.2.4.5 void register_signal_handlers ( )

Tie various signal handlers to Dakota's abort_handler function.

Global function to register signal handlers at top-level.

References abort_handler().

Referenced by main().

13.2.4.6 void mpi_debug_hold ( )

Global function to hold Dakota processes to help with MPI debugging.

See details in code for details, depending on MPI implementation in use.

Referenced by main().

13.2.4.7 T Dakota::abort_handler_t (int *code*)

Templatized abort_handler_t method that allows for convenient return from methods that otherwise have no sensible return from error clauses. Usage: MyType& method() { return abort_handler<MyType&>(-1); }

References abort_handler().

13.2.4.8 void svd (RealMatrix & *matrix,* RealVector & *singular_vals,* RealMatrix & *v_trans,* bool *compute_vectors* = true)

Compute the SVD of an arbitrary matrix A = USV^T.

Uses Teuchos::LAPACK.GESVD() to compute the singular value decomposition, overwriting A with the left singular vectors U (or destroying A if compute_vectors = false); optionally returns right singular vectors in v_trans.

References abort_handler().

Referenced by ProbabilityTransformModel::acv_index_to_corr_index(), Model::assign_max_strings(), NonDBayesCalibration::augment_gradient_with_log_prior(), NonDBayesCalibration::augment_hessian_with_log_prior(), NonDAdaptImpSampling::calculate_statistics(), PebbldBranchSub::candidateSolution(), ActiveSubspaceModel::compute_bing_li_criterion(), ActiveSubspaceModel::compute_constantine_metric(), ActiveSubspaceModel::compute_svd(), Variables::continuous_variable_id(), Variables::continuous_variable_ids(), Variables::continuous_variable_label(), Variables::continuous_variable_labels(), Variables::continuous_variable_type(), Variables::continuous_variable_types(), SharedVariablesData::copy(), Model::discrete_int_sets(), Variables::discrete_int_variable_label(), Variables::discrete_int_variable_labels(), Variables::discrete_int_variable_type(), Variables::discrete_int_variable_types(), Variables::discrete_real_variable_label(), Variables::discrete_real_variable_labels(), Variables::discrete_real_variable_type(), Variables::discrete_real_variable_types(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Variables::discrete_string_variable_label(), Variables::discrete_string_variable_labels(), Variables::discrete_string_variable_type(), Variables::discrete_string_variable_types(), ParamStudy::distribute(), QMEApproximation::find_scaled_coefficients(), NonDAdaptImpSampling::generate_samples(), Constraints::get_constraints(), DataTransformModel::get_hyperparam_vc_index(), Variables::inactive_continuous_variable_ids(), Variables::inactive_continuous_variable_labels(), Variables::inactive_continuous_variable_types(), Variables::inactive_discrete_int_variable_labels(), Variables::inactive_discrete_int_variable_types(), Variables::inactive_discrete_real_variable_labels(), Variables::inactive_discrete_real_variable_types(), Variables::inactive_discrete_string_variable_labels(), Variables::inactive_discrete_string_variable_types(), NonDLHSSampling::increm_lhs_parameter_set(), DataTransformModel::init_continuous_vars(), RecastModel::init_variables(), SimulationModel::initialize_solution_control(), MinimizerAdapterModel::initialize_variables(), ExperimentData::load_data(), NonDSampling::mode_bits(), NonDSampling::mode_counts(), NestedModel::NestedModel(), NonDInterval::NonDInterval(), NonDLHSSampling::NonDLHSSampling(), Optimizer::Optimizer(), SensAnalysisGlobal::partial_corr(), ParamStudy::pre_run(), NonDBayesCalibration::prior_sample(), ProbabilityTransformModel::ProbabilityTransformModel(), NonDAdaptImpSampling::recentered_density(), Constraints::reshape(), SubspaceModel::resize_variable_totals(), NonDSampling::sample_to_variables(), NonDAdaptImpSampling::select_rep_points(), singular_values(), PebbldBranchSub::splitComputation(), SubspaceModel::uncertain_vars_to_subspace(), SurrogateModel::update_distributions_from_model(), NonDExpansion::update_final_statistics_gradients(), SurrogateModel::update_model_distributions(), NestedModel::update_sub_model(), ReducedBasis::update_svd(), DataTransformModel::variables_expand(), RandomFieldModel::variables_resize(), and NonDSampling::variables_to_sample().

13.2.4.9 int qr (RealMatrix & *A*)

Compute an in-place QR factorization A = QR.

Uses Teuchos::LAPACK.GEQRF() to compute the QR decomposition, overwriting A with the transformations and R.

References abort_handler().

Referenced by SensAnalysisGlobal::partial_corr().

13.2.4.10 int qr_rsolve (const RealMatrix & *q_r,* bool *transpose,* RealMatrix & *rhs*)

Perform a multiple right-hand sides Rinv $*$ rhs solve using the R from a qr factorization.

Returns info $>$ 0 if the matrix is singular

Uses Teuchos::LAPACK.TRTRS() to perform a triangular backsolve

References abort_handler().

Referenced by SensAnalysisGlobal::partial_corr().

13.2.4.11 int generate_system_seed ( )

clock microseconds-based random seed in [1, 1000000]

Mimics DDACE timeSeed(), which returns the trailing microseconds on the time of day clock. Historically, most algorithms opted for DDACE, Utilib, std::clock(), in that order.

Referenced by NonDWASABIBayesCalibration::calibrate(), PSUADEDesignCompExp::get_parameter_sets(), F-SUDesignCompExp::get_parameter_sets(), NonDQuadrature::get_parameter_sets(), NonDSampling::initialize_-sample_driver(), and NonDBayesCalibration::NonDBayesCalibration().

13.2.4.12 bool Dakota::operator!= (const ActiveSet & *set1,* const ActiveSet & *set2*) [inline]

inequality operator for ActiveSet

inequality operator

13.2.4.13 bool Dakota::operator== (const Model & *m1,* const Model & *m2*) [inline]

equality operator for Envelope is true if same letter instance

equality operator (detect same letter instance)

References Model::modelRep.

13.2.4.14 bool Dakota::operator!= (const Model & *m1,* const Model & *m2*) [inline]

inequality operator for Envelope is true if different letter instance

inequality operator (detect different letter instances)

References Model::modelRep.

13.2.4.15 void Dakota::get_initial_values (const Model & *model,* VecT & *values*)

Adapter for copying initial continuous variables values from a Dakota Model into TPL vectors

References Model::continuous_variables(), and Model::cv().

Referenced by ROLOptimizer::set_problem().

13.2.4.16 bool Dakota::get_bounds (const RealVector & *lower_source,* const RealVector & *upper_source,* VecT & *lower_target,* VecT & *upper_target,* Real *big_real_bound_size,* Real *no_value*)

Adapter for copying continuous variables data from Dakota RealVector into TPL vectors

Referenced by get_linear_constraints(), get_variable_bounds(), and ROLOptimizer::set_problem().

13.2.4.17 void Dakota::get_bounds (const Model & *model,* VecT & *lower_target,* VecT & *upper_target*)

Adapter for copying continuous variables data from a Dakota Model into TPL vectors

References Model::continuous_lower_bounds(), and Model::continuous_upper_bounds().

13.2.4.18 void Dakota::get_bounds (const SetT & *source_set,* VecT & *lower_target,* VecT & *upper_target,* int *target_offset*)

Adapter originating from (and somewhat specialized based on) APPSOptimizer for copying discrete variables from a set-based Dakota container into TPL vectors

13.2.4.19 bool Dakota::get_mixed_bounds (const MaskType & *mask_set,* const SetArray & *source_set,* const Teuchos::SerialDenseVector< OrdinalType, ScalarType > & *lower_source,* const Teuchos::SerialDenseVector< OrdinalType, ScalarType > & *upper_source,* VectorType2 & *lower_target,* VectorType2 & *upper_target,* ScalarType *bigBoundSize,* ScalarType *no_value,* int *target_offset =* `0`)

Adapter originating from (and somewhat specialized based on) APPSOptimizer for copying discrete integer variables data with bit masking from Dakota into TPL vectors

Referenced by get_variable_bounds().

13.2.4.20 bool Dakota::get_variable_bounds (Model & *model,* Real *big_real_bound_size,* int *big_int_bound_size,* typename AdapterT::VecT & *lower,* typename AdapterT::VecT & *upper*)

Adapter originating from (and somewhat specialized based on) APPSOptimizer for copying heterogeneous bounded data from Dakota::Variables into concatenated TPL vectors

References Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::cv(), Model::discrete_int_lower_bounds(), Model::discrete_int_sets(), Model::discrete_int_upper_bounds(), Model::discrete_real_lower_bounds(), Model::discrete_real_upper_bounds(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Model::div(), Model::drv(), get_bounds(), and get_mixed_bounds().

13.2.4.21 int Dakota::configure_inequality_constraint_maps (const Model & *model,* Real *big_real_bound_size,* CONSTRAINT_TYPE *ctype,* IVecT & *map_indices,* RVecT & *map_multipliers,* RVecT & *map_offsets,* Real *scaling =* `1.0`)

Adapter for configuring inequality constraint maps used when transferring data between Dakota and a TPL

References Model::linear_ineq_constraint_lower_bounds(), Model::linear_ineq_constraint_upper_bounds(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Model::num_linear_ineq_constraints(), and Model::num_nonlinear_ineq_constraints().

Referenced by Optimizer::configure_constraint_maps().

13.2.4.22 void Dakota::configure_equality_constraint_maps (Model & *model,* CONSTRAINT_TYPE *ctype,* IVecT & *indices,* size_t *index_offset,* RVecT & *multipliers,* RVecT & *values,* bool *make_one_sided*)

Adapter for configuring equality constraint maps used when transferring data between Dakota and a TPL

References Model::linear_eq_constraint_targets(), Model::nonlinear_eq_constraint_targets(), Model::num_linear_eq_constraints(), and Model::num_nonlinear_eq_constraints().

13.2.4.23 void Dakota::get_linear_constraints (Model & *model,* Real *big_real_bound_size,* typename AdapterT::VecT & *lin_ineq_lower_bnds,* typename AdapterT::VecT & *lin_ineq_upper_bnds,* typename AdapterT::VecT & *lin_eq_targets,* typename AdapterT::MatT & *lin_ineq_coeffs,* typename AdapterT::MatT & *lin_eq_coeffs*)

Adapter based initially on APPSOptimizer for linear constraint maps and including matrix and bounds data; bundles a few steps together which could (should?) be broken into two or more adapters

References copy_data(), get_bounds(), Model::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_targets(), Model::linear_ineq_constraint_coeffs(), Model::linear_ineq_constraint_lower_bounds(), and Model::linear_ineq_constraint_upper_bounds().

13.2.4.24 void Dakota::apply_linear_constraints (const Model & *model,* CONSTRAINT_EQUALITY_TYPE *etype,* const VecT & *in_vals,* VecT & *values,* bool *adjoint* = `false`)

Data adapter to transfer data from Dakota to third-party opt packages. The vector values might contain additional constraints; the first entries corresponding to linear constraints are populated by apply.

References apply_matrix_partial(), Model::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_targets(), Model::linear_ineq_constraint_coeffs(), Model::num_linear_eq_constraints(), and Model::num_linear_ineq_constraints().

Referenced by DakotaROLIneqConstraints::value(), and DakotaROLEqConstraints::value().

13.2.4.25 void Dakota::apply_nonlinear_constraints (const Model & *model,* CONSTRAINT_EQUALITY_TYPE *etype,* const VecT & *in_vals,* VecT & *values,* bool *adjoint* = `false`)

Data adapter to transfer data from Dakota to third-party opt packages

If adjoint = false, (perhaps counter-intuitively) apply the Jacobian (transpose of the gradient) to in_vals, which should be of size num_continuous_vars: $J*x = G'*x$, resulting in num_nonlinear_const values getting populated (possibly a subset of the total constraint vector).

If adjoint = true, apply the adjoint Jacobian (gradient) to the nonlinear constraint portion of in_vals, which should be of size at least num_nonlinear_consts: $J'*y = G*y$, resulting in num_continuous_vars values getting populated.

References Model::current_response(), Model::cv(), Response::function_gradients(), Model::num_linear_eq_constraints(), Model::num_linear_ineq_constraints(), Model::num_nonlinear_eq_constraints(), and Model::num_nonlinear_ineq_constraints().

Referenced by DakotaROLIneqConstraintsGrad::applyAdjointJacobian(), DakotaROLEqConstraintsGrad::applyAdjointJacobian(), DakotaROLIneqConstraintsGrad::applyJacobian(), and DakotaROLEqConstraintsGrad::applyJacobian().

13.2.4.26 void Dakota::set_best_responses (typename AdapterT::OptT & *optimizer,* const Model & *model,* bool *set_objectives,* size_t *num_user_primary_fns,* const std::vector< int > *constraint_map_indices,* const std::vector< double > *constraint_map_multipliers,* const std::vector< double > *constraint_map_offsets,* ResponseArray & *response_array*)

Data adapter for use by third-party opt packages to transfer response data to Dakota

References Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), and Model::primary_response_fn_sense().

13.2.4.27 void Dakota::set_variables (const VectorType & *source,* Model & *model,* Variables & *vars*)

copy appropriate slices of source vector to Dakota::Variables

References Variables::continuous_variables(), copy_data_partial(), Variables::cv(), Model::discrete_int_sets(), Variables::discrete_int_variables(), Variables::discrete_real_variables(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Variables::discrete_string_variable(), Variables::div(), Variables::drv(), Variables::dsv(), and set_index_to_value().

Referenced by NomadOptimizer::Evaluator::eval_x().

13.2.4.28 void Dakota::get_variables (Model & *model,* VectorType & *vec*)

copy the various pieces comprising Dakota::Variables into a concatenated TPL vector

References abort_handler(), Model::continuous_variables(), copy_data_partial(), Model::cv(), Model::discrete_int_sets(), Model::discrete_int_variables(), Model::discrete_real_variables(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Model::discrete_string_variables(), Model::div(), Model::drv(), and Model::dsv().

13.2.4.29 void Dakota::get_responses (const Model & *model,* const RealVector & *dak_fn_vals,* const std::vector< int > *constraint_map_indices,* const std::vector< double > *constraint_map_multipliers,* const std::vector< double > *constraint_map_offsets,* vectorType & *f_vec,* vectorType & *cEqs_vec,* vectorType & *cIneqs_vec*)

Data adapter to transfer data from Dakota to third-party opt packages

References Model::num_nonlinear_eq_constraints(), and Model::primary_response_fn_sense().

Referenced by NomadOptimizer::Evaluator::eval_x(), and Optimizer::get_responses_from_dakota().

13.2.4.30 void Dakota::get_nonlinear_eq_constraints (const Model & *model,* VecT & *values,* Real *scale,* int *offset* = -1)

Data adapter to transfer data from Dakota to third-party opt packages

References Model::current_response(), Response::function_values(), Model::nonlinear_eq_constraint_targets(), Model::num_linear_eq_constraints(), Model::num_nonlinear_eq_constraints(), and Model::num_nonlinear_ineq_constraints().

Referenced by DakotaROLEqConstraints::value().

13.2.4.31 void Dakota::get_nonlinear_eq_constraints (Model & *model,* const RealVector & *curr_resp_vals,* VecT & *values,* Real *scale,* int *offset* = 0)

Data adapter to transfer data from Dakota to third-party opt packages

References Model::nonlinear_eq_constraint_targets(), and Model::num_nonlinear_eq_constraints().

13.2.4.32 void Dakota::get_nonlinear_ineq_constraints (const Model & *model,* VecT & *values*)

Data adapter to transfer data from Dakota to third-party opt packages (ROL-specific)

References copy_data_partial(), Model::current_response(), Response::function_values(), Model::num_linear_ineq_constraints(), and Model::num_nonlinear_ineq_constraints().

Referenced by DakotaROLIneqConstraints::value().

13.2.4.33 void Dakota::get_nonlinear_bounds (Model & *model,* VecT & *nonlin_ineq_lower,* VecT & *nonlin_ineq_upper,* VecT & *nonlin_eq_targets*)

Would like to combine the previous adapter with this one (based on APPSOptimizer and COLINOptimizer) and then see how much more generalization is needed to support other TPLs like JEGA.

Data adapter to transfer data from Dakota to third-party opt packages

References copy_data(), Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_lower_-bounds(), and Model::nonlinear_ineq_constraint_upper_bounds().

Referenced by COLINApplication::set_problem().

13.2.4.34 bool Dakota::operator!= (const Response & *resp1,* const Response & *resp2*) [inline]

inequality operator for Response

inequality operator

13.2.4.35 bool Dakota::operator!= (const Variables & *vars1,* const Variables & *vars2*) [inline]

inequality operator for Variables

strict inequality operator

13.2.4.36 void Dakota::write_ordered (std::ostream & *s,* const SizetArray & *comp_totals,* const Teuchos::SerialDenseVector< OrdinalType, ScalarType1 > & *c_vector,* const Teuchos::SerialDenseVector< OrdinalType, ScalarType2 > & *di_vector,* const Teuchos::SerialDenseVector< OrdinalType, ScalarType3 > & *ds_vector,* const Teuchos::SerialDenseVector< OrdinalType, ScalarType4 > & *dr_vector*) [inline]

free function to write Variables data vectors in input spec ordering

written for arbitrary types, but typical use will be ScalarType1 = Real, ScalarType2 = int, ScalarType3 = string, and ScalarType4 = int or Real.

Referenced by ParamStudy::pre_run().

13.2.4.37 void Dakota::write_ordered (std::ostream & *s,* const SizetArray & *comp_totals,* const Teuchos::SerialDenseVector< OrdinalType, ScalarType1 > & *c_vector,* const Teuchos::SerialDenseVector< OrdinalType, ScalarType2 > & *di_vector,* const boost::multi_array< ScalarType3, 1 > & *ds_array,* const Teuchos::SerialDenseVector< OrdinalType, ScalarType4 > & *dr_vector*) [inline]

free function to write Variables data vectors in input spec ordering

written for arbitrary types, but typical use will be ScalarType1 = Real, ScalarType2 = int, ScalarType3 = string, and ScalarType4 = int or Real.

13.2.4.38 void copy_field_data (const RealVector & *fn_vals,* RealMatrix & *fn_grad,* const RealSymMatrixArray & *fn_hess,* size_t *offset,* size_t *num_fns,* Response & *response*)

This assumes the souce gradient/Hessian are size less or equal to the destination response, and that the leading part is to be populated.

References Response::active_set_request_vector(), Response::function_gradient_view(), Response::function_-hessian_view(), and Response::function_value().

Referenced by ExperimentData::scale_residuals().

13.2.4.39 void Dakota::copy_field_data (const RealVector & *fn_vals,* RealMatrix & *fn_grad,* const RealSymMatrixArray & *fn_hess,* size_t *offset,* size_t *num_fns,* short *total_asv,* Response & *response*)

This assumes the souce gradient/Hessian are size less or equal to the destination response, and that the leading part is to be populated.

References Response::function_gradient_view(), Response::function_hessian_view(), and Response::function_-value().

13.2.4.40 void symmetric_eigenvalue_decomposition (const RealSymMatrix & *matrix,* RealVector & *eigenvalues,* RealMatrix & *eigenvectors*)

Computes the eigenvalues and, optionally, eigenvectors of a real symmetric matrix A.

Eigenvalues are returned in ascending order.

References symmetric_eigenvalue_decomposition().

Referenced by NonDBayesCalibration::get_positive_definite_covariance_from_hessian(), and symmetric_-eigenvalue_decomposition().

13.2.4.41 Real Dakota::getdist (const RealVector & *x1,* const RealVector & *x2*)

Gets the Euclidean distance between x1 and x2

Referenced by mindist(), and mindistindx().

13.2.4.42 Real Dakota::mindist (const RealVector & *x,* const RealMatrix & *xset,* int *except*)

Returns the minimum distance between the point x and the points in the set xset (compares against all points in xset except point "except"): if except is not needed, pass 0.

References getdist().

Referenced by getRmax().

13.2.4.43 Real Dakota::mindistindx (const RealVector & *x,* const RealMatrix & *xset,* const IntArray & *indx*)

Gets the min distance between x and points in the set xset defined by the nindx values in indx.

References getdist().

Referenced by GaussProcApproximation::pointsel_add_sel().

13.2.4.44 Real Dakota::getRmax (const RealMatrix & *xset*)

Gets the maximum of the min distance between each point and the rest of the set.

References mindist().

Referenced by GaussProcApproximation::pointsel_add_sel().

13.2.4.45 int Dakota::start_grid_computing (char ∗ *analysis_driver_script,* char ∗ *params_file,* char ∗ *results_file*)

sample function prototype for launching grid computing

13.2.4.46 int Dakota::stop_grid_computing ( )

sample function prototype for terminating grid computing

13.2.4.47 int Dakota::perform_analysis (char * *iteration_num*)

sample function prototype for submitting a grid evaluation

13.2.4.48 string Dakota::asstring (const T & *val*)

Creates a string from the argument *val* using an ostringstream.

This only gets used in this file and is only ever called with ints so no error checking is in place.

Parameters

val	The value of type T to convert to a string.

Returns

The string representation of *val* created using an ostringstream.

Referenced by JEGAOptimizer::LoadTheConstraints().

13.2.4.49 void start_dakota_heartbeat (int *seconds*)

Heartbeat function provided by dakota_filesystem_utils; pass output interval in seconds, or -1 to use $DAKOTA_H-EARTBEAT

Referenced by OutputManager::OutputManager().

13.2.4.50 bool Dakota::operator== (const ParamResponsePair & *pair1,* const ParamResponsePair & *pair2*) [inline]

equality operator for ParamResponsePair

equality operator

References ParamResponsePair::evalInterfaceIds, ParamResponsePair::prpResponse, and ParamResponsePair-::prpVariables.

13.2.4.51 bool Dakota::operator!= (const ParamResponsePair & *pair1,* const ParamResponsePair & *pair2*) [inline]

inequality operator for ParamResponsePair

inequality operator

13.2.4.52 bool Dakota::set_compare (const ParamResponsePair & *database_pr,* const ActiveSet & *search_set*) [inline]

search function for a particular ParamResponsePair within a PRPList based on ActiveSet content (request vector and derivative variables vector)

a global function to compare the ActiveSet of a particular database_pr (presumed to be in the global history list) with a passed in ActiveSet (search_set).

References ParamResponsePair::active_set(), ActiveSet::derivative_vector(), and ActiveSet::request_vector().

Referenced by lookup_by_val().

13.2.4.53 bool Dakota::id_vars_exact_compare (const ParamResponsePair & *database_pr,* const ParamResponsePair & *search_pr*) [inline]

search function for a particular ParamResponsePair within a PRPMultiIndex a global function to compare the interface id and variables of a particular database_pr (presumed to be in the global history list) with a passed in key of interface id and variables provided by search_pr.

References ParamResponsePair::interface_id(), and ParamResponsePair::variables().

Referenced by partial_prp_equality::operator()().

13.2.4.54 PRPCacheHIter Dakota::lookup_by_val (PRPMultiIndexCache & *prp_cache,* const ParamResponsePair & *search_pr*) [inline]

find a ParamResponsePair based on the interface id, variables, and ActiveSet search data within search_pr.

Lookup occurs in two steps: (1) PRPMultiIndexCache lookup based on strict equality in interface id and variables, and (2) set_compare() post-processing based on ActiveSet subset logic.

References ParamResponsePair::active_set(), and set_compare().

Referenced by NonDDREAMBayesCalibration::archive_acceptance_chain(), Minimizer::archive_best_results(), DataTransformModel::archive_submodel_responses(), NonDMUQBayesCalibration::cache_chain(), NonDQUESOBayesCalibration::cache_chain(), Model::db_lookup(), ApplicationInterface::duplication_detect(), SurrBasedLocalMinimizer::find_response(), Minimizer::local_recast_retrieve(), lookup_by_val(), Minimizer::print_best_eval_ids(), DiscrepancyCorrection::search_db(), and NonDLocalReliability::update_mpp_search_data().

13.2.4.55 PRPQueueHIter Dakota::lookup_by_val (PRPMultiIndexQueue & *prp_queue,* const ParamResponsePair & *search_pr*) [inline]

find a ParamResponsePair based on the interface id, variables, and ActiveSet search data within search_pr.

Lookup occurs in two steps: (1) PRPMultiIndexQueue lookup based on strict equality in interface id and variables, and (2) set_compare() post-processing based on ActiveSet subset logic.

References ParamResponsePair::active_set(), and set_compare().

13.2.4.56 void print_restart (StringArray *pos_args,* String *print_dest*)

print a restart file

Usage: "dakota_restart_util print dakota.rst"

"dakota_restart_util to_neutral dakota.rst dakota.neu"

Prints all evals. in full precision to either stdout or a neutral file. The former is useful for ensuring that duplicate detection is successful in a restarted run (e.g., starting a new method from the previous best), and the latter is used for translating binary files between platforms.

References abort_handler(), ParamResponsePair::eval_id(), ParamResponsePair::write_annotated(), and write_precision.

Referenced by main().

13.2.4.57 void print_restart_pdb (StringArray *pos_args,* String *print_dest*)

print a restart file (PDB format)

Usage: "dakota_restart_util to_pdb dakota.rst dakota.pdb"

Unrolls all data associated with a particular tag for all evaluations and then writes this data in a tabular format (e.g., to a PDB database or MATLAB/TECPLOT data file).

References abort_handler(), Variables::continuous_variables(), Variables::discrete_int_variables(), Variables::discrete_real_variables(), and Response::function_values().

Referenced by main().

13.2.4.58 void print_restart_tabular (StringArray *pos_args,* String *print_dest,* unsigned short *tabular_format,* int *tabular_precision*)

print a restart file (tabular format)

Usage: "dakota_restart_util to_tabular dakota.rst dakota.txt"

Unrolls all data associated with a particular tag for all evaluations and then writes this data in a tabular format (e.g., to a PDB database or MATLAB/TECPLOT data file).

References abort_handler(), Variables::acv(), Variables::adiv(), Variables::adrv(), Variables::adsv(), Variables::all_continuous_variable_labels(), Variables::all_discrete_int_variable_labels(), Variables::all_discrete_real_variable_labels(), Variables::all_discrete_string_variable_labels(), Response::function_labels(), ParamResponsePair::interface_id(), ParamResponsePair::response(), ParamResponsePair::variables(), write_precision, ParamResponsePair::write_tabular(), and ParamResponsePair::write_tabular_labels().

Referenced by main().

13.2.4.59 void read_neutral (StringArray *pos_args*)

read a restart file (neutral file format)

Usage: "dakota_restart_util from_neutral dakota.neu dakota.rst"

Reads evaluations from a neutral file. This is used for translating binary files between platforms.

References abort_handler(), and ParamResponsePair::read_annotated().

Referenced by main().

13.2.4.60 void repair_restart (StringArray *pos_args,* String *identifier_type*)

repair a restart file by removing corrupted evaluations

Usage: "dakota_restart_util remove 0.0 dakota_old.rst dakota_new.rst"

"dakota_restart_util remove_ids 2 7 13 dakota_old.rst dakota_new.rst"

Repairs a restart file by removing corrupted evaluations. The identifier for evaluation removal can be either a double precision number (all evaluations having a matching response function value are removed) or a list of integers (all evaluations with matching evaluation ids are removed).

References abort_handler(), Response::active_set_request_vector(), contains(), ParamResponsePair::eval_id(), Response::function_values(), and ParamResponsePair::response().

Referenced by main().

13.2.4.61 void concatenate_restart (StringArray *pos_args*)

concatenate multiple restart files

Usage: "dakota_restart_util cat dakota_1.rst ... dakota_n.rst dakota_new.rst"

Combines multiple restart files into a single restart database.

References abort_handler().

Referenced by main().

13.2.4.62 std::vector<std::string> Dakota::get_pathext ( )

Utility function for executable file search algorithms

Referenced by WorkdirHelper::which().

13.2.4.63 bool Dakota::contains (const bfs::path & *dir_path*, const std::string & *file_name*, boost::filesystem::path & *complete_filepath*) [inline]

Utility function for "which" sets complete_filepath from dir_path/file_name combo

13.2.5 Variable Documentation

13.2.5.1 short abort_mode = ABORT_EXITS

by default Dakota exits or calls MPI_Abort on errors

whether dakota exits/aborts or throws on errors

Referenced by abort_throw_or_exit(), Environment::exit_mode(), and PythonInterface::python_run().

13.2.5.2 UShortStrBimap submethod_map [static]

Initial value:

```
=
  boost::assign::list_of<UShortStrBimap::relation>
  (HYBRID,                         "hybrid")
  (SUBMETHOD_COLLABORATIVE,        "collaborative")
  (SUBMETHOD_EMBEDDED,             "embedded")
  (SUBMETHOD_SEQUENTIAL,           "sequential")
  (SUBMETHOD_LHS,                  "lhs")
  (SUBMETHOD_RANDOM,               "random")
  (SUBMETHOD_BOX_BEHNKEN,          "box_behnken")
  (SUBMETHOD_CENTRAL_COMPOSITE,    "central_composite")
  (SUBMETHOD_GRID,                 "grid")
  (SUBMETHOD_OA_LHS,               "oa_lhs")
  (SUBMETHOD_OAS,                  "oas")
  (SUBMETHOD_ACV_IS,               "acv_is")
  (SUBMETHOD_ACV_MF,               "acv_mf")
  (SUBMETHOD_ACV_KL,               "acv_kl")
  (SUBMETHOD_DREAM,                "dream")
  (SUBMETHOD_WASABI,               "wasabi")
  (SUBMETHOD_GPMSA,                "gpmsa")
  (SUBMETHOD_MUQ,                  "muq")
  (SUBMETHOD_QUESO,                "queso")
  (SUBMETHOD_OPTPP,                "nip")
  (SUBMETHOD_NPSOL,                "sqp")
  (SUBMETHOD_EA,                   "ea")
  (SUBMETHOD_EGO,                  "ego")
  (SUBMETHOD_SBGO,                 "sbgo")
  (SUBMETHOD_CONVERGE_ORDER,       "converge_order")
  (SUBMETHOD_CONVERGE_QOI,         "converge_qoi")
  (SUBMETHOD_ESTIMATE_ORDER,       "estimate_order")
```

bimap between sub-method enums and strings; only used in this compilation unit (using bimap for consistency, though at time of addition, only uni-directional mapping is supported)

Referenced by Iterator::submethod_enum_to_string().

13.2.5.3 Dakota_funcs DakFuncs0

Initial value:

```
= {
        fprintf,
        abort_handler,
        dlsolver_option,
        continuous_lower_bounds1,
        continuous_upper_bounds1,
        nonlinear_ineq_constraint_lower_bounds1,
        nonlinear_ineq_constraint_upper_bounds1,
        nonlinear_eq_constraint_targets1,
        linear_ineq_constraint_lower_bounds1,
        linear_ineq_constraint_upper_bounds1,
        linear_eq_constraint_targets1,
```

```
        linear_ineq_constraint_coeffs1,
        linear_eq_constraint_coeffs1,
        ComputeResponses1,
        GetFuncs1,
        GetGrads1,
        GetContVars1,
        SetBestContVars1,
        SetBestDiscVars1,
        SetBestRespFns1,
        Get_Real1,
        Get_Int1,
        Get_Bool1
        }
```

13.2.5.4 const char∗ FIELD_NAMES[ ]

Initial value:

```
= { "numFns", "numVars", "numACV", "numADIV",
                              "numADRV", "numDerivVars", "xC", "xDI",
                              "xDR", "xCLabels", "xDILabels",
                              "xDRLabels", "directFnASV", "directFnDVV",
                              "fnFlag", "gradFlag", "hessFlag",
                              "fnVals",  "fnGrads",  "fnHessians",
                              "fnLabels", "failure", "currEvalId" }
```

fields to pass to Matlab in Dakota structure

Referenced by MatlabInterface::matlab_engine_run(), and MatlabInterface::MatlabInterface().

13.2.5.5 const int NUMBER_OF_FIELDS = 23

number of fields in above structure

Referenced by MatlabInterface::matlab_engine_run(), and MatlabInterface::MatlabInterface().

13.2.5.6 Var_uinfo CAUVLbl[CAUVar_Nkinds] [static]

Initial value:

```
= {
  VarLabelInfo(nuv_, NormalUnc),
  VarLabelInfo(lnuv_, LognormalUnc),
  VarLabelInfo(uuv_, UniformUnc),
  VarLabelInfo(luuv_, LoguniformUnc),
  VarLabelInfo(tuv_, TriangularUnc),
  VarLabelInfo(euv_, ExponentialUnc),
  VarLabelInfo(beuv_, BetaUnc),
  VarLabelInfo(gauv_, GammaUnc),
  VarLabelInfo(guuv_, GumbelUnc),
  VarLabelInfo(fuv_, FrechetUnc),
  VarLabelInfo(wuv_, WeibullUnc),
  VarLabelInfo(hbuv_, HistogramBinUnc)
}
```

13.2.5.7 Var_uinfo DAUIVLbl[DAUIVar_Nkinds] [static]

Initial value:

```
= {
  VarLabelInfo(puv_, PoissonUnc),
  VarLabelInfo(biuv_, BinomialUnc),
  VarLabelInfo(nbuv_, NegBinomialUnc),
  VarLabelInfo(geuv_, GeometricUnc),
  VarLabelInfo(hguv_, HyperGeomUnc),
  VarLabelInfo(hpiuv_, HistogramPtIntUnc)
}
```

13.2.5.8 Var_uinfo DAUSVLbl[DAUSVar_Nkinds] [static]

Initial value:

```
= {
  VarLabelInfo(hpsuv_, HistogramPtStrUnc)
}
```

13.2.5.9 Var_uinfo DAURVLbl[DAURVar_Nkinds] [static]

Initial value:

```
= {
  VarLabelInfo(hpruv_, HistogramPtRealUnc)
}
```

13.2.5.10 Var_uinfo CEUVLbl[CEUVar_Nkinds] [static]

Initial value:

```
= {
  VarLabelInfo(ciuv_, ContinuousIntervalUnc)
}
```

13.2.5.11 Var_uinfo DEUIVLbl[DEUIVar_Nkinds] [static]

Initial value:

```
= {
  VarLabelInfo(diuv_, DiscreteIntervalUnc),
  VarLabelInfo(dusiv_, DiscreteUncSetInt)
}
```

13.2.5.12 Var_uinfo DEUSVLbl[DEUSVar_Nkinds] [static]

Initial value:

```
= {
  VarLabelInfo(dussv_, DiscreteUncSetStr)
}
```

13.2.5.13 Var_uinfo DEURVLbl[DEURVar_Nkinds] [static]

Initial value:

```
= {
  VarLabelInfo(dusrv_, DiscreteUncSetReal)
}
```

13.2.5.14 Var_uinfo DiscSetLbl[DiscSetVar_Nkinds] [static]

Initial value:

```
= {
  VarLabelInfo(ddsiv_, DiscreteDesSetInt),
  VarLabelInfo(ddssv_, DiscreteDesSetStr),
  VarLabelInfo(ddsrv_, DiscreteDesSetReal),
  VarLabelInfo(dssiv_, DiscreteStateSetInt),
  VarLabelInfo(dsssv_, DiscreteStateSetStr),
  VarLabelInfo(dssrv_, DiscreteStateSetReal)
}
```

13.2.5.15 VarLabelChk DesignAndStateLabelsCheck[ ] [static]

Initial value:

```
= {
  { AVI numContinuousDesVars, AVI continuousDesignLabels, "cdv_", "cdv_descriptors" },
  { AVI numDiscreteDesRangeVars, AVI discreteDesignRangeLabels, "ddriv_", "ddriv_descriptors" },
  { AVI numDiscreteDesSetIntVars, AVI discreteDesignSetIntLabels, "ddsiv_", "ddsiv_descriptors" },
  { AVI numDiscreteDesSetStrVars, AVI discreteDesignSetStrLabels, "ddssv_", "ddssv_descriptors" },
  { AVI numDiscreteDesSetRealVars, AVI discreteDesignSetRealLabels, "ddsrv_", "ddsrv_descriptors" },
  { AVI numContinuousStateVars, AVI continuousStateLabels, "csv_", "csv_descriptors" },
  { AVI numDiscreteStateRangeVars, AVI discreteStateRangeLabels, "dsriv_", "dsriv_descriptors" },
  { AVI numDiscreteStateSetIntVars, AVI discreteStateSetIntLabels, "dssiv_", "dssiv_descriptors" },
  { AVI numDiscreteStateSetStrVars, AVI discreteStateSetStrLabels, "dsssv_", "dsssv_descriptors" },
  { AVI numDiscreteStateSetRealVars, AVI discreteStateSetRealLabels, "dssrv_", "dssrv_descriptors" },
  { AVI numContinuousDesVars, AVI continuousDesignScaleTypes, 0, "cdv_scale_types" }
}
```

Variables label array designations for design and state. All non-uncertain variables need to be in this array. Used in check_variables_node to check lengths and make_variable_defaults to build labels.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_-defaults().

13.2.5.16 VLreal VLUncertainReal[NUM_UNC_REAL_CONT] [static]

Initial value:

```
= {
 {CAUVar_Nkinds,  AVI CAUv,  CAUVLbl,
        DVR continuousAleatoryUncLabels,
        DVR continuousAleatoryUncLowerBnds,
        DVR continuousAleatoryUncUpperBnds,
        DVR continuousAleatoryUncVars},
 {CEUVar_Nkinds,  AVI CEUv,  CEUVLbl,
        DVR continuousEpistemicUncLabels,
        DVR continuousEpistemicUncLowerBnds,
        DVR continuousEpistemicUncUpperBnds,
        DVR continuousEpistemicUncVars},
 {DAURVar_Nkinds, AVI DAURv, DAURVLbl,
        DVR discreteRealAleatoryUncLabels,
        DVR discreteRealAleatoryUncLowerBnds,
        DVR discreteRealAleatoryUncUpperBnds,
        DVR discreteRealAleatoryUncVars},
 {DEURVar_Nkinds, AVI DEURv, DEURVLbl,
        DVR discreteRealEpistemicUncLabels,
        DVR discreteRealEpistemicUncLowerBnds,
        DVR discreteRealEpistemicUncUpperBnds,
        DVR discreteRealEpistemicUncVars}}
```

Variables labels/bounds/values check array for real-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., CAUVLbl, with the contiguous container in which they are stored.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_-defaults().

13.2.5.17 VLint VLUncertainInt[NUM_UNC_INT_CONT] [static]

Initial value:

```
= {
 {DAUIVar_Nkinds, AVI DAUIv, DAUIVLbl,
        DVR discreteIntAleatoryUncLabels,
        DVR discreteIntAleatoryUncLowerBnds,
        DVR discreteIntAleatoryUncUpperBnds,
        DVR discreteIntAleatoryUncVars},
 {DEUIVar_Nkinds, AVI DEUIv, DEUIVLbl,
        DVR discreteIntEpistemicUncLabels,
        DVR discreteIntEpistemicUncLowerBnds,
        DVR discreteIntEpistemicUncUpperBnds,
        DVR discreteIntEpistemicUncVars}}
```

Variables labels/bounds/values check array for integer-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., DAUIVLbl, with the contiguous container in which they are stored.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_-defaults().

13.2.5.18 VLstr VLUncertainStr[NUM_UNC_STR_CONT] [static]

Initial value:

```
= {
 {DAUSVar_Nkinds, AVI DAUSv, DAUSVLbl,
        DVR discreteStrAleatoryUncLabels,
        DVR discreteStrAleatoryUncLowerBnds,
        DVR discreteStrAleatoryUncUpperBnds,
        DVR discreteStrAleatoryUncVars},
 {DEUSVar_Nkinds, AVI DEUSv, DEUSVLbl,
        DVR discreteStrEpistemicUncLabels,
        DVR discreteStrEpistemicUncLowerBnds,
        DVR discreteStrEpistemicUncUpperBnds,
        DVR discreteStrEpistemicUncVars}}
```

Variables labels/bounds/values check array for string-valued uncertain variables; one array entry per contiguous container. These associate the individual variables given by, e.g., DAUSVLbl, with the contiguous container in which they are stored.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_-defaults().

13.2.5.19 Var_check var_mp_check_cv[ ] [static]

Initial value:

```
= {
        Vchk_3(continuous_design,ContinuousDes),
        Vchk_3(continuous_state,ContinuousState) }
```

13.2.5.20 Var_check var_mp_check_dset[ ] [static]

Initial value:

```
= {
        Vchk_3(discrete_design_set_integer,DiscreteDesSetInt),
        Vchk_3(discrete_design_set_string,DiscreteDesSetStr),
        Vchk_3(discrete_design_set_real,DiscreteDesSetReal),
        Vchk_3(discrete_state_set_integer,DiscreteStateSetInt),
        Vchk_3(discrete_state_set_string,DiscreteStateSetStr),
        Vchk_3(discrete_state_set_real,DiscreteStateSetReal) }
```

13.2.5.21 Var_check var_mp_check_cau[ ] [static]

Initial value:

```
= {
        Vchk_3(normal_uncertain,NormalUnc),
        Vchk_3(lognormal_uncertain,LognormalUnc),
        Vchk_3(uniform_uncertain,UniformUnc),
        Vchk_3(loguniform_uncertain,LoguniformUnc),
        Vchk_3(triangular_uncertain,TriangularUnc),
        Vchk_3(exponential_uncertain,ExponentialUnc),
        Vchk_3(beta_uncertain,BetaUnc),
        Vchk_3(gamma_uncertain,GammaUnc),
        Vchk_3(gumbel_uncertain,GumbelUnc),
        Vchk_3(frechet_uncertain,FrechetUnc),
        Vchk_3(weibull_uncertain,WeibullUnc),
        Vchk_3(histogram_bin_uncertain,HistogramBinUnc) }
```

13.2.5.22 Var_check var_mp_check_daui[ ] [static]

Initial value:

```
= {
        Vchk_3(poisson_uncertain,PoissonUnc),
        Vchk_3(binomial_uncertain,BinomialUnc),
        Vchk_3(negative_binomial_uncertain,NegBinomialUnc),
        Vchk_3(geometric_uncertain,GeometricUnc),
        Vchk_3(hypergeometric_uncertain,HyperGeomUnc),
        Vchk_3(histogram_point_int_uncertain,HistogramPtIntUnc) }
```

13.2.5.23 Var_check var_mp_check_daus[ ] [static]

Initial value:

```
= {
        Vchk_3(histogram_point_str_uncertain,HistogramPtStrUnc) }
```

13.2.5.24 Var_check var_mp_check_daur[ ] [static]

Initial value:

```
= {
        Vchk_3(histogram_point_real_uncertain,HistogramPtRealUnc) }
```

13.2.5.25 Var_check var_mp_check_ceu[ ] [static]

Initial value:

```
= {
        Vchk_3(continuous_interval_uncertain,ContinuousIntervalUnc) }
```

13.2.5.26 Var_check var_mp_check_deui[ ] [static]

Initial value:

```
= {
        Vchk_3(discrete_interval_uncertain,DiscreteIntervalUnc),
        Vchk_3(discrete_uncertain_set_integer,DiscreteUncSetInt) }
```

13.2.5.27 Var_check var_mp_check_deus[ ] [static]

Initial value:

```
= {
        Vchk_3(discrete_uncertain_set_string,DiscreteUncSetStr) }
```

13.2.5.28 Var_check var_mp_check_deur[ ] [static]

Initial value:

```
= {
        Vchk_3(discrete_uncertain_set_real,DiscreteUncSetReal) }
```

13.2.5.29 Var_rcheck var_mp_cbound[ ] [static]

Initial value:

```
= {
        Vchk_7(continuous_design,ContinuousDes,continuousDesign),
        Vchk_7(continuous_state,ContinuousState,continuousState),


        Vchk_5(normal_uncertain,NormalUnc,normalUnc),
        Vchk_5(lognormal_uncertain,LognormalUnc,lognormalUnc),
        Vchk_5(uniform_uncertain,UniformUnc,uniformUnc),
        Vchk_5(loguniform_uncertain,LoguniformUnc,loguniformUnc),
        Vchk_5(triangular_uncertain,TriangularUnc,triangularUnc),
        Vchk_5(beta_uncertain,BetaUnc,betaUnc) }
```

This is used within check_variables_node(): Var_RealBoundIPCheck() is applied to validate bounds and initial points.

Referenced by NIDRProblemDescDB::check_variables_node().

13.2.5.30 Var_icheck var_mp_drange[ ] [static]

Initial value:

```
= {
        Vchk_7(discrete_design_range,DiscreteDesRange,discreteDesignRange),
        Vchk_7(discrete_state_range,DiscreteStateRange,discreteStateRange) }
```

This is used in check_variables_node(): Var_IntBoundIPCheck() is applied to validate bounds and initial points, and in make_variable_defaults(): Vgen_∗ is called to infer bounds.

Referenced by NIDRProblemDescDB::check_variables_node(), and NIDRProblemDescDB::make_variable_-defaults().

13.2.5.31 const char∗ SCI_FIELD_NAMES[ ]

Initial value:

```
= { "dakota_type", "numFns", "numVars", "numACV", "numADIV",
                                  "numADRV", "numDerivVars", "xC", "xDI",
                                  "xDR", "xCLabels", "xDILabels",
                                  "xDRLabels", "directFnASV", "directFnASM",
                                  "directFnDVV", "directFnDVV_bool",
                                  "fnFlag", "gradFlag", "hessFlag",
                                  "fnVals",  "fnGrads",  "fnHessians",
                                  "fnLabels", "failure", "currEvalId" }
```

fields to pass to Scilab in Dakota structure

Referenced by ScilabInterface::scilab_engine_run().

13.2.5.32 const int SCI_NUMBER_OF_FIELDS = 26

number of fields in above structure

Referenced by ScilabInterface::scilab_engine_run().

13.3 dakota::surrogates Namespace Reference

namespace for new Dakota surrogates module

Classes

- class Surrogate

    Parent class for surrogate models.
- class GaussianProcess

    The GaussianProcess constructs a Gaussian Process regressor surrogate given a matrix of data.
- class Kernel

    Kernel functions for the Gaussian Process surrogate.
- class SquaredExponentialKernel

    Stationary kernel with C^ smooth realizations.
- class Matern32Kernel

    Stationary kernel with C^1 smooth realizations.
- class Matern52Kernel

    Stationary kernel with C^2 smooth realizations.
- class GP_Objective

    ROL objective function for the Gaussian Process (GP) surrogate.
- class PolynomialRegression

    The PolynomialRegression class constructs a polynomial regressor using ordinary least squares.

Typedefs

- using RolVec = ROL::Vector< double >

    Dakota alias for ROL Vector.
- using RolStdVec = ROL::StdVector< double >

    Dakota alias for ROL StdVector.
- using SCALER_TYPE = util::DataScaler::SCALER_TYPE

    alias for util SCALER_TYPE enum
- using SOLVER_TYPE = util::LinearSolverBase::SOLVER_TYPE

    alias for util SOLVER_TYPE enum

Functions

- void compute_next_combination (int num_dims, int level, VectorXi &index, bool &extend, int &h, int &t)
- void size_level_index_vector (int num_dims, int level, MatrixXi &indices)

    Compute a matrix of basis indices for given dimension and level. Each row of the matrix sums to level.
- void compute_hyperbolic_subdim_level_indices (int num_dims, int level, int num_active_dims, double p, MatrixXi &indices)

    Compute a matrix of indices for a submatrix (i.e. up to the active dimensions column) of indices produced by size_level_index_vector(num_dims, level, indices) where each feature has a component > 0 and respects the p-norm cutoff.
- void compute_hyperbolic_level_indices (int num_dims, int level, double p, MatrixXi &indices)

    Compute the hyperbolic cross indices for a given level.
- void compute_hyperbolic_indices (int num_dims, int level, double p, MatrixXi &indices)

    Compute the hyperbolic cross indices for all levels up to level.
- void compute_reduced_indices (int num_dims, int level, MatrixXi &indices)

    Compute the reduced indices for all levels up to level.
- void fd_check_gradient (Surrogate &surr, const MatrixXd &sample, MatrixXd &fd_error, const int num_steps=10)

    Perform a centered finite difference check of a Surrogate's gradient method.
- void fd_check_hessian (Surrogate &surr, const MatrixXd &sample, MatrixXd &fd_error, const int num_steps=10)

Perform a centered finite difference check of a Surrogate's Hessian method.
- std::vector< MatrixXd > compute_cw_dists_squared (const std::vector< MatrixXd > &cw_dists)

  Compute a vector of component-wise squared distances from a vector of component-wise signed distances.
- std::shared_ptr< Kernel > kernel_factory (const std::string &kernel_type)

  Creates a derived Kernel class.

13.3.1 Detailed Description

namespace for new Dakota surrogates module

13.3.2 Function Documentation

13.3.2.1 void compute_next_combination (int *num_dims,* int *level,* VectorXi & *index,* bool & *extend,* int & *h,* int & *t*)

Parameters

in	*num_dims*	Dimension of the feature space.
in	*level*	Total order in each row of indices. Should be >= 1.
in,out	*index*	Vector of ints that specifies the powers for each term in the basis.
in,out	*extend*	Bool for whether to continue with the computation of basis indices.
in,out	*h*	Working variable for basis enumeration.
in,out	*t*	Working variable for basis enumeration.

Referenced by size_level_index_vector().

13.3.2.2 void size_level_index_vector (int *num_dims,* int *level,* MatrixXi & *indices*)

Compute a matrix of basis indices for given dimension and level. Each row of the matrix sums to level.

Parameters

in	*num_dims*	Dimension of the feature space.
in	*level*	Total order in each row of indices. Should be >= 1.
out	*indices*	Matrix of indices - (num_terms by num_dims).

References compute_next_combination(), and dakota::util::n_choose_k().

Referenced by compute_hyperbolic_level_indices(), and compute_hyperbolic_subdim_level_indices().

13.3.2.3 void compute_hyperbolic_subdim_level_indices (int *num_dims,* int *level,* int *num_active_dims,* double *p,* MatrixXi & *indices*)

Compute a matrix of indices for a submatrix (i.e. up to the active dimensions column) of indices produced by size_level_index_vector(num_dims, level, indices) where each feature has a component > 0 and respects the p-norm cutoff.

Parameters

in	*num_dims*	Dimension of the feature space.
in	*level*	Total order in each row of indices. Should be >= 1.
in	*num_active_dims*	The # of active features and end index of the submatrix.

in	*p*	Real value for p-norm.
out	*indices*	Matrix of indices - (num_terms by num_active_dims)

References dakota::util::num_nonzeros(), dakota::util::p_norm(), dakota::silence_unused_args(), and size_level_-index_vector().

Referenced by compute_hyperbolic_level_indices().

13.3.2.4 void compute_hyperbolic_level_indices (int *num_dims,* int *level,* double *p,* MatrixXi & *indices*)

Compute the hyperbolic cross indices for a given level.

Parameters

in	*num_dims*	Dimension of the feature space.
in	*level*	Total order in each column of indices. Should be >= 0.
in	*p*	Real value for p-norm.
out	*indices*	Matrix of indices - (num_dims by num_terms)

References dakota::util::append_columns(), compute_hyperbolic_subdim_level_indices(), dakota::util::nonzero(), dakota::util::num_nonzeros(), and size_level_index_vector().

Referenced by compute_hyperbolic_indices().

13.3.2.5 void compute_hyperbolic_indices (int *num_dims,* int *level,* double *p,* MatrixXi & *indices*)

Compute the hyperbolic cross indices for all levels up to level.

Parameters

in	*num_dims*	Dimension of the feature space.
in	*level*	Highest level to compute basis indices for.
in	*p*	Real value for p-norm.
out	*indices*	Matrix of indices - (num_dims by num_terms).

References dakota::util::append_columns(), and compute_hyperbolic_level_indices().

Referenced by PolynomialRegression::build().

13.3.2.6 void compute_reduced_indices (int *num_dims,* int *level,* MatrixXi & *indices*)

Compute the reduced indices for all levels up to level.

Parameters

in	*num_dims*	Dimension of the feature space.
in	*level*	Highest level to compute basis indices for.
out	*indices*	Matrix of indices - (num_dims by num_terms).

References dakota::util::append_columns().

Referenced by PolynomialRegression::build().

13.3.2.7 void fd_check_gradient (Surrogate & *surr,* const MatrixXd & *sample,* MatrixXd & *fd_error,* const int *num_steps* = 10)

Perform a centered finite difference check of a Surrogate's gradient method.

Parameters

in	*surr*	Reference to a Surrogate.
in	*sample*	Point to evaluate the gradient at - (1 by numVariables).
out	*fd_error*	Matrix of finite difference error for each component of the gradient - (num_-steps by numVariables).
in	*num_steps*	Number of increments (N) for the finite difference. The increment vector h = 10∗∗(-i), i = 1, ..., N.

References Surrogate::dataScaler, DataScaler::get_scaler_features_scale_factors(), Surrogate::gradient(), and Surrogate::value().

13.3.2.8 void fd_check_hessian (Surrogate & *surr*, const MatrixXd & *sample*, MatrixXd & *fd_error*, const int *num_steps* = `10`)

Perform a centered finite difference check of a Surrogate's Hessian method.

Parameters

in	*surr*	Reference to a Surrogate.
in	*sample*	Point to evaluate the Hessian at - (1 by numVariables).
out	*fd_error*	Matrix of finite difference error for each independent component of the Hessian. There are numVariables∗(numVariables+1)/2 = numInd components - (num_steps by numInd). of the Hessian - (num_steps by numVariables).
in	*num_steps*	Number of increments (N) for the finite difference. The increment vector h = 10∗∗(-i), i = 1, ..., N.

References Surrogate::dataScaler, DataScaler::get_scaler_features_scale_factors(), Surrogate::hessian(), and Surrogate::value().

13.3.2.9 std::vector< MatrixXd > compute_cw_dists_squared (const std::vector< MatrixXd > & *cw_dists*)

Compute a vector of component-wise squared distances from a vector of component-wise signed distances.

Parameters

in	*dists2*	Vector of signed component-wise distances.

Returns

Vector of squared distances.

Referenced by Matern32Kernel::compute_first_deriv_pred_gram(), Matern52Kernel::compute_first_deriv_pred_-gram(), and Matern52Kernel::compute_second_deriv_pred_gram().

13.3.2.10 std::shared_ptr< Kernel > kernel_factory (const std::string & *kernel_type*)

Creates a derived Kernel class.

Parameters

in	*kernel_type*	Name of the kernel.

Returns

Pointer to specialized kernel class.

Referenced by GaussianProcess::build(), and GaussianProcess::serialize().

13.4 dakota::util Namespace Reference

namespace for new Dakota utilities module

Classes

- class DataScaler

  The DataScaler class computes the scaling coefficients and scales a 2D data matrix with dimensions num_samples by num_features.
- class NormalizationScaler

  Normalizes the data using max and min feature values.
- class StandardizationScaler

  Standardizes the data so the each feature has zero mean and unit variance.
- class NoScaler

  Leaves the data unscaled.
- class LinearSolverBase

  The LinearSolverBase class serves as an API for derived solvers.
- class LUSolver

  The LUSolver class is used to solve linear systems with the LU decomposition.
- class SVDSolver

  The SVDSolver class is used to solve linear systems with the singular value decomposition.
- class QRSolver

  The QRSolver class solves the linear least squares problem with a QR decomposition.
- class CholeskySolver

  The CholeskySolver class is used to solve linear systems with a symmetric matrix with a pivoted Cholesky decomposition.

Typedefs

- using BimapMetrictypeStr = boost::bimap< METRIC_TYPE, std::string >

  alias for Boost Bimap metric type <–> string
- using SCALER_TYPE = DataScaler::SCALER_TYPE

  alias for DataScaler's SCALER_TYPE
- using BimapScalertypeStr = boost::bimap< SCALER_TYPE, std::string >

  alias for Boost Bimap scaler type <–> string
- using SOLVER_TYPE = LinearSolverBase::SOLVER_TYPE

  alias for LinearSolverBase's SOLVER_TYPE
- using BimapSolvertypeStr = boost::bimap< SOLVER_TYPE, std::string >

  alias for Boost Bimap solver type <–> string

Enumerations

- enum METRIC_TYPE {
  SUM_SQUARED, **MEAN_SQUARED**, **ROOT_MEAN_SQUARED**, **SUM_ABS**,
  MEAN_ABS, **MAX_ABS**, **ABS_PERCENTAGE_ERROR**, **MEAN_ABS_PERCENTAGE_ERROR**,
  R_SQUARED }

  Enumeration for supported metric types.

Functions

- void error (const std::string &msg)

  Throws a std::runtime_error based on the message argument.
- bool matrix_equals (const MatrixXi &A, const MatrixXi &B)

  Tests whether two Eigen MatrixXi objects are equal.
- bool matrix_equals (const MatrixXd &A, const MatrixXd &B, double tol)

  Tests whether two Eigen MatrixXd objects are equal, within a given tolerance.
- bool matrix_equals (const RealMatrix &A, const RealMatrix &B, double tol)

  Tests whether two Teuchos RealMatrix objects are equal, within a given tolerance.
- bool relative_allclose (const MatrixXd &A, const MatrixXd &B, const double tol)

  Tests whether two Eigen MatrixXd objects relatively equal (element-wise) within a given tolerance.
- double variance (const VectorXd &vec)

  Calculates the variance based on an Eigen VectorXd of double values.
- void populateVectorsFromFile (const std::string &filename, std::vector< VectorXd > &R, int num_datasets, int num_samples)

  Populate a collection of vectors read in a from a text file assuming data layout is one dataset per row.
- void populateMatricesFromFile (const std::string &filename, std::vector< MatrixXd > &S, int num_datasets, int num_vars, int num_samples)

  Populate a collection of matrices read in a from a text file assuming data layout is a "column-major" stack of num_-samples by num_vars matrices.
- int n_choose_k (int n, int k)

  Calculate Binomial coefficient n choose k.
- void random_permutation (const int num_pts, const unsigned int seed, VectorXi &permutations)

  Random permutation of int array.
- void create_cv_folds (const int num_folds, const int num_pts, std::vector< VectorXi > &fold_indices, const int seed=22)

  Generate indices for cross validation folds.
- MatrixXd create_uniform_random_double_matrix (const int rows, const int cols)

  Generate a real-valued matrix of uniformly distributed random values.
- MatrixXd create_uniform_random_double_matrix (const int rows, const int cols, const unsigned int seed)

  Generate a real-valued matrix of uniformly distributed random values.
- MatrixXd create_uniform_random_double_matrix (const int rows, const int cols, const unsigned int seed, bool transform, const double low, const double high)

  Generate a real-valued matrix of uniformly distributed random values.
- template<typename T >
  int num_nonzeros (const T &mat)

  Caclulate and return number of nonzero entries in vector or matrix.
- template<typename T1 , typename T2 >
  void nonzero (const T1 &v, T2 &result)

  Create a vector of indices based on nonzero entries in input vector.
- template<typename T1 , typename T2 >
  void append_columns (const T1 &new_cols, T2 &target)

  Append columns of input matrix to existing matrix.
- template<typename T >
  double p_norm (const T &v, double p)

  Caclulate and return p-norm of a vector.
- METRIC_TYPE metric_type (const std::string &metric_name)

  Convert the metric from string to enum.
- double compute_metric (const VectorXd &p, const VectorXd &d, const std::string &metric_name)

  Computes the difference between prediction and data vectors.
- std::shared_ptr< DataScaler > scaler_factory (DataScaler::SCALER_TYPE scaler_type, const MatrixXd &unscaled_matrix)

Free function to construct DataScaler.

- std::shared_ptr< LinearSolverBase > solver_factory (LinearSolverBase::SOLVER_TYPE type)

  Free function to construct LinearSolverBase.

Variables

- static BimapMetrictypeStr type_name_bimap

  Bimap between metric types and names.
- static BimapScalertypeStr type_name_bimap

  Bimap between scaler types and names.
- static BimapSolvertypeStr type_name_bimap

  Bimap between solver types and names.

13.4.1 Detailed Description

namespace for new Dakota utilities module

13.4.2 Function Documentation

13.4.2.1 void error (const std::string & *msg*)

Throws a std::runtime_error based on the message argument.

Parameters

in	*msg*	The error message to throw

Referenced by compute_metric(), create_cv_folds(), and matrix_equals().

13.4.2.2 bool matrix_equals (const MatrixXi & *A*, const MatrixXi & *B*)

Tests whether two Eigen MatrixXi objects are equal.

Parameters

in	*A*	The first matrix to test
in	*B*	The second matrix to test

Returns

Whether the matrices are equal

13.4.2.3 bool matrix_equals (const MatrixXd & *A*, const MatrixXd & *B*, double *tol*)

Tests whether two Eigen MatrixXd objects are equal, within a given tolerance.

Parameters

in	*A*	The first matrix to test
in	*B*	The second matrix to test

in	*tol*	The tolerance to use when comparing double values

Returns

Whether the matrices are equal to within tolerance

References error().

13.4.2.4 bool matrix_equals (const RealMatrix & *A*, const RealMatrix & *B*, double *tol*)

Tests whether two Teuchos RealMatrix objects are equal, within a given tolerance.

Parameters

in	*A*	The first matrix to test
in	*B*	The second matrix to test
in	*tol*	The tolerance to use when comparing double values

Returns

Whether the matrices are equal to within tolerance

References error().

13.4.2.5 bool relative_allclose (const MatrixXd & *A*, const MatrixXd & *B*, const double *tol*)

Tests whether two Eigen MatrixXd objects relatively equal (element-wise) within a given tolerance.

Parameters

in	*A*	The first matrix to test
in	*B*	The second matrix to test
in	*tol*	The relative tolerance to use when comparing double values

Returns

Whether the matrices are relatively equal (within the tolerance)

13.4.2.6 double variance (const VectorXd & *vec*)

Calculates the variance based on an Eigen VectorXd of double values.

Parameters

in	*vec*	The vector

Returns

The calculated variance

13.4.2.7 void populateVectorsFromFile (const std::string & *filename*, std::vector< VectorXd > & *R*, int *num_datasets*, int *num_samples*)

Populate a collection of vectors read in a from a text file assuming data layout is one dataset per row.

Parameters

in	*filename*	The file that contains the data
out	*R*	The collection of vectors to be populated
in	*num_datasets*	The number of datasets to read in
in	*num_samples*	The number of data points (e.g. function values, build points) per dataset

13.4.2.8 void populateMatricesFromFile (const std::string & *filename,* std::vector< MatrixXd > & *S,* int *num_datasets,* int *num_vars,* int *num_samples*)

Populate a collection of matrices read in a from a text file assuming data layout is a "column-major" stack of num_-samples by num_vars matrices.

Parameters

in	*filename*	The file that contains the data
out	*S*	The collection of vectors to be populated
in	*num_datasets*	The number of datasets to read in
in	*num_samples*	The number of data points (e.g. function values, build points) per dataset (row dim)
in	*num_vars*	The number of variables per dataset (column dim)

13.4.2.9 int n_choose_k (int *n,* int *k*)

Calculate Binomial coefficient n choose k.

Parameters

in	*n*	Number of elements in set
in	*k*	Number of elements in subset k where n >= k >= 0

Returns

Number of ways to choose an (unordered) subset of k elements from a fixed set of n elements

Referenced by dakota::surrogates::size_level_index_vector().

13.4.2.10 int dakota::util::num_nonzeros (const T & *mat*)

Caclulate and return number of nonzero entries in vector or matrix.

Parameters

in	*mat*	Incoming vector or matrix

Returns

Number of nonzeros

Referenced by dakota::surrogates::compute_hyperbolic_level_indices(), dakota::surrogates::compute_hyperbolic_-subdim_level_indices(), and nonzero().

13.4.2.11 void dakota::util::nonzero (const T1 & *v,* T2 & *result*)

Create a vector of indices based on nonzero entries in input vector.

Parameters

in	*v*	Incoming vector
out	*result*	Vector having values at nonzero locations of incoming vector and value equal to ordinal of occurrence

References num_nonzeros().

Referenced by dakota::surrogates::compute_hyperbolic_level_indices().

13.4.2.12 void dakota::util::append_columns (const T1 & *new_cols,* T2 & *target*)

Append columns of input matrix to existing matrix.

Parameters

in	*new_cols*	Incoming matrix of column vectors to append
out	*target*	Matrix to augment with appended columns

Referenced by dakota::surrogates::compute_hyperbolic_indices(), dakota::surrogates::compute_hyperbolic_level_-indices(), and dakota::surrogates::compute_reduced_indices().

13.4.2.13 double dakota::util::p_norm (const T & *v,* double *p*)

Caclulate and return p-norm of a vector.

Parameters

in	*v*	Incoming vector
in	*p*	Order or norm to compute

Returns

p-norm of incoming vector

Referenced by dakota::surrogates::compute_hyperbolic_subdim_level_indices().

13.4.2.14 METRIC_TYPE metric_type (const std::string & *metric_name*)

Convert the metric from string to enum.

Parameters

in	*metric_name*	metric

Returns

converted metric

References type_name_bimap.

Referenced by compute_metric().

13.4.2.15 double compute_metric (const VectorXd & *p,* const VectorXd & *d,* const std::string & *metric_name*)

Computes the difference between prediction and data vectors.

Parameters

in	*p*	prediction vector.
in	*d*	data vector.
in	*metric_name*	metric to compute.

Returns

the value of the computed metric.

References error(), and metric_type().

Referenced by Surrogate::evaluate_metrics().

13.4.2.16 std::shared_ptr< DataScaler > scaler_factory (DataScaler::SCALER_TYPE *scaler_type*, const MatrixXd & *unscaled_matrix*)

Free function to construct DataScaler.

Parameters

in	*scaler_type*	Which scaler to construct
in	*unscaled_matrix*	Unscaled data matrix - (num_samples by num_features)

Returns

Shared pointer to a DataScaler

Referenced by PolynomialRegression::build(), and GaussianProcess::build().

13.4.2.17 std::shared_ptr< LinearSolverBase > solver_factory (LinearSolverBase::SOLVER_TYPE *type*)

Free function to construct LinearSolverBase.

Parameters

in	*type*	Which solver to construct

Returns

Shared pointer to a LinearSolverBase

Referenced by PolynomialRegression::build().

13.4.3 Variable Documentation

13.4.3.1 BimapMetrictypeStr type_name_bimap [static]

Initial value:

```
=
    boost::assign::list_of<BimapMetrictypeStr::relation>

    (METRIC_TYPE::SUM_SQUARED, "sum_squared")
    (METRIC_TYPE::MEAN_SQUARED, "mean_squared")
    (METRIC_TYPE::ROOT_MEAN_SQUARED, "root_mean_squared")
    (METRIC_TYPE::SUM_ABS, "sum_abs")
    (METRIC_TYPE::MEAN_ABS, "mean_abs")
    (METRIC_TYPE::MAX_ABS, "max_abs")
    (METRIC_TYPE::ABS_PERCENTAGE_ERROR, "ape")
    (METRIC_TYPE::MEAN_ABS_PERCENTAGE_ERROR, "mape")
    (METRIC_TYPE::R_SQUARED, "rsquared")
```

Bimap between metric types and names.

Referenced by metric_type(), DataScaler::scaler_type(), and LinearSolverBase::solver_type().

13.4.3.2 BimapScalertypeStr type_name_bimap [static]

Initial value:

```
=
    boost::assign::list_of<BimapScalertypeStr::relation>

    (SCALER_TYPE::NONE, "none")
    (SCALER_TYPE::STANDARDIZATION, "standardization")
    (SCALER_TYPE::MEAN_NORMALIZATION, "mean normalization")
    (SCALER_TYPE::MINMAX_NORMALIZATION, "min-max normalization")
```

Bimap between scaler types and names.

13.4.3.3 BimapSolvertypeStr type_name_bimap [static]

Initial value:

```
=
    boost::assign::list_of<BimapSolvertypeStr::relation>

    (SOLVER_TYPE::CHOLESKY, "cholesky")
    (SOLVER_TYPE::EQ_CONS_LEAST_SQ_REGRESSION, "equality-constrained lsq regression")
    (SOLVER_TYPE::LASSO_REGRESSION, "lasso regression")
    (SOLVER_TYPE::LEAST_ANGLE_REGRESSION, "least angle regression")
    (SOLVER_TYPE::LU, "LU")
    (SOLVER_TYPE::ORTHOG_MATCH_PURSUIT, "orthogonal matching pursuit")
    (SOLVER_TYPE::QR_LEAST_SQ_REGRESSION, "QR lsq regression")
    (SOLVER_TYPE::SVD_LEAST_SQ_REGRESSION, "SVD")
```

Bimap between solver types and names.

13.5 SIM Namespace Reference

A sample namespace for derived classes that use assign_rep() to plug facilities into DAKOTA.

Classes

- class ParallelDirectApplicInterface

  Sample derived interface class for testing parallel simulator plug-ins using assign_rep().
- class SerialDirectApplicInterface

  Sample derived interface class for testing serial simulator plug-ins using assign_rep().

13.5.1 Detailed Description

A sample namespace for derived classes that use assign_rep() to plug facilities into DAKOTA. A typical use of plug-ins with assign_rep() is to publish a simulation interface for use in library mode See Interfacing with Dakota as a Library for more information.

13.6 StanfordPSAAP Namespace Reference

A sample namespace for derived classes that use assign_rep() to plug facilities into DAKOTA.

Classes

- class SoleilDirectApplicInterface

  Sample derived interface class for testing serial simulator plug-ins using assign_rep().

13.6.1 Detailed Description

A sample namespace for derived classes that use assign_rep() to plug facilities into DAKOTA. A typical use of plug-ins with assign_rep() is to publish a simulation interface for use in library mode See Interfacing with Dakota as a Library for more information.

Chapter 14

Class Documentation

14.1 ActiveSet Class Reference

Container class for active set tracking information. Contains the active set request vector and the derivative variables vector.

Public Member Functions

- ActiveSet ()

    default constructor
- ActiveSet (size_t num_fns, size_t num_deriv_vars)

    standard constructor
- ActiveSet (size_t num_fns)

    partial constructor
- ActiveSet (const ShortArray &asv, const SizetArray &dvv)

    alt constructor
- ActiveSet (const ActiveSet &set)

    copy constructor
- ∼ActiveSet ()

    destructor
- ActiveSet & operator= (const ActiveSet &set)

    assignment operator
- void reshape (size_t num_fns, size_t num_deriv_vars)

    reshape requestVector and derivVarsVector
- void reshape (size_t num_fns)

    reshape requestVector
- const ShortArray & request_vector () const

    return the request vector
- ShortArray & request_vector ()

    return the request vector
- void request_vector (const ShortArray &rv)

    set the request vector
- void request_values (const short rv_val)

    set all request vector values
- void request_values (const short rv_val, size_t start, size_t end)

    set all request vector values in a range
- short request_value (const size_t index) const

get the value of an entry in the request vector
- void request_value (const short rv_val, const size_t index)

  set the value of an entry in the request vector
- const SizetArray & derivative_vector () const

  return the derivative variables vector
- SizetArray & derivative_vector ()

  return the derivative variables vector
- void derivative_vector (const SizetArray &dvv)

  set the derivative variables vector from a SizetArray
- void derivative_vector (SizetMultiArrayConstView dvv)

  set the derivative variables vector from a SizetMultiArrayConstView
- void derivative_start_value (size_t dvv_start_val)

  set the derivative variables vector values
- void read (std::istream &s)

  read an active set object from an std::istream
- void write (std::ostream &s) const

  write an active set object to an std::ostream
- void write_annotated (std::ostream &s) const

  write an active set object to an std::ostream in annotated format
- void read (MPIUnpackBuffer &s)

  read an active set object from a packed MPI buffer
- void write (MPIPackBuffer &s) const

  write an active set object to a packed MPI buffer

Private Member Functions

- template<class Archive >
  void serialize (Archive &ar, const unsigned int version)

  implementation of Boost serialize for ActiveSet

Private Attributes

- ShortArray requestVector

  the vector of response requests
- SizetArray derivVarsVector

  the vector of variable ids used for computing derivatives

Friends

- class **boost::serialization::access**
- bool operator== (const ActiveSet &set1, const ActiveSet &set2)

  equality operator
- bool operator!= (const ActiveSet &set1, const ActiveSet &set2)

  inequality operator

14.1.1 Detailed Description

Container class for active set tracking information. Contains the active set request vector and the derivative variables vector.

The ActiveSet class is a small class whose initial design function is to avoid having to pass the ASV and DV-V separately. It is not part of a class hierarchy and does not employ reference-counting/ representation-sharing idioms (e.g., handle-body).

14.1.2 Member Data Documentation

14.1.2.1 ShortArray requestVector [private]

the vector of response requests

It uses a 0 value for inactive functions and sums 1 (value), 2 (gradient), and 4 (Hessian) for active functions.

Referenced by ActiveSet::ActiveSet(), ActiveSet::operator=(), ActiveSet::read(), ActiveSet::request_value(), ActiveSet::request_values(), ActiveSet::request_vector(), ActiveSet::reshape(), ActiveSet::write(), and ActiveSet::write_annotated().

14.1.2.2 SizetArray derivVarsVector [private]

the vector of variable ids used for computing derivatives

These ids will generally identify either the active continuous variables or the inactive continuous variables.

Referenced by ActiveSet::ActiveSet(), ActiveSet::derivative_start_value(), ActiveSet::derivative_vector(), ActiveSet::operator=(), ActiveSet::read(), ActiveSet::reshape(), ActiveSet::write(), and ActiveSet::write_annotated().

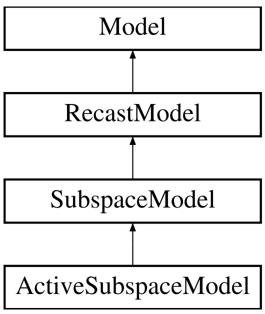
The documentation for this class was generated from the following file:

- DakotaActiveSet.hpp

14.2 ActiveSubspaceModel Class Reference

Active subspace model for input (variable space) reduction.

Inheritance diagram for ActiveSubspaceModel:



Public Member Functions

- ActiveSubspaceModel (ProblemDescDB &problem_db)

  Problem database constructor.
- ActiveSubspaceModel (const Model &sub_model, unsigned int dimension, const RealMatrix &rotation_matrix, short output_level)

  lightweight constructor
- ∼ActiveSubspaceModel ()

  destructor

Protected Member Functions

- void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)
- void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)

portion of set_communicators() specific to derived model classes
- void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)

  portion of free_communicators() specific to derived model classes
- void derived_evaluate (const ActiveSet &set)

  portion of evaluate() specific to derived model classes
- void derived_evaluate_nowait (const ActiveSet &set)

  portion of evaluate_nowait() specific to derived model classes
- const IntResponseMap & derived_synchronize ()

  portion of synchronize() specific to derived model classes
- const IntResponseMap & derived_synchronize_nowait ()

  portion of synchronize_nowait() specific to derived model classes
- void validate_inputs ()

  validate the build controls and set defaults
- void assign_instance ()

  assign static pointer instance to this for use in static transformation functions
- Model get_sub_model (ProblemDescDB &problem_db)

  retrieve the sub-Model from the DB to pass up the constructor chain
- void init_fullspace_sampler (unsigned short sample_type)

  initialize the native problem space Monte Carlo sampler
- void compute_subspace ()

  sample the model's gradient, computed the SVD, and form the active subspace rotation matrix.
- void initialize_subspace ()

  helper for shared code between lightweight ctor and initialize_mapping()
- void generate_fullspace_samples (unsigned int diff_samples)

  sample the derivative at diff_samples points and leave temporary in dace_iterator
- void populate_matrices (unsigned int diff_samples)

  populate the derivative and vars matrices with fullspaceSampler samples
- void compute_svd ()

  factor the derivative matrix and analyze singular values, assessing convergence and rank, returning whether tolerance met
- void truncate_subspace ()

  use the truncation methods to identify the size of an active subspace
- unsigned int compute_bing_li_criterion (RealVector &singular_values)

  compute Bing Li's criterion to identify the active subspace
- unsigned int compute_constantine_metric (RealVector &singular_values)

  compute Constantine's metric to identify the active subspace
- unsigned int compute_energy_criterion (RealVector &singular_values)

  Compute active subspace size based on eigenvalue energy. Compatible with other truncation methods.
- unsigned int compute_cross_validation_metric ()

  Use cross validation of a moving least squares surrogate to identify the size of an active subspace that meets an error tolerance.
- Real build_cv_surrogate (Model &cv_surr_model, RealMatrix training_x, IntResponseMap training_y, RealMatrix test_x, IntResponseMap test_y)

  Build moving least squares surrogate over candidate active subspace.
- unsigned int **determine_rank_cv** (const std::vector< Real > &cv_error)
- unsigned int **min_index** (const std::vector< Real > &cv_error)
- unsigned int **tolerance_met_index** (const std::vector< Real > &cv_error, Real tolerance, bool &tol_met)
- std::vector< Real > **negative_diff** (const std::vector< Real > &cv_error)
- void build_surrogate ()

  Build surrogate over active subspace.
- SizetArray resize_variable_totals ()

  Create a variables components totals array with the reduced space size for continuous variables.
- void uncertain_vars_to_subspace ()

  translate the characterization of uncertain variables in the native_model to the reduced space of the transformed model

Static Protected Member Functions

- static void variables_mapping (const Variables &recast_xi_vars, Variables &sub_model_x_vars)

  map the active continuous recast variables to the active submodel variables (linear transformation)

Protected Attributes

- int initialSamples

  initial number of samples at which to query the truth model
- bool subspaceIdBingLi

  Boolean flag signaling use of Bing Li criterion to identify active subspace dimension.
- bool subspaceIdConstantine

  Boolean flag signaling use of Constantine criterion to identify active subspace dimension.
- bool subspaceIdEnergy

  Boolean flag signaling use of eigenvalue energy criterion to identify active subspace dimension.
- bool subspaceIdCV

  Boolean flag signaling use of cross validationto identify active subspace dimension.
- size_t numReplicates

  Number of bootstrap samples for subspace identification.
- bool transformVars

  boolean flag to determine if variables should be transformed to u-space before active subspace initialization
- unsigned int totalSamples

  total construction samples evaluated so far
- unsigned short subspaceNormalization

  Normalization to use in the case of multiple QoI's.
- RealMatrix inactiveBasis

  basis for the inactive subspace
- RealVector inactiveVars

  current inactive variables
- RealMatrix derivativeMatrix

  matrix of derivative data with numFns columns per fullspace sample; each column contains the gradient of one function at one sample point, so total matrix size is numContinuousVars $*$ (numFns $*$ numSamples) [D1 | D2 | ... | Dnum_samples] [dy1/dx(k=1) | dy2/dx(k=1) | ... | dyM/dx(k=1) | k=2 | ... | k=n_s]
- RealMatrix leftSingularVectors

  matrix of the left singular vectors of derivativeMatrix
- RealVector singularValues

  singular values of derivativeMatrix
- RealMatrix varsMatrix

  matrix of fullspace variable points samples size numContinuousVars $*$ (numSamples)
- RealArray gradientScaleFactors

  Gradient scaling factors to make multiple response function gradients similar orders of magnitude.
- Real truncationTolerance

  Truncation tolerance for eigenvalue energy subspace identification.
- bool **cvIncremental**
- short **cvIdMethod**
- Real **cvRelTolerance**
- Real **cvDecreaseTolerance**
- unsigned int cvMaxRank

  maximum subspace size to consider using cross validation
- Model surrogateModel

  model containing a surrogate built over the active subspace

- bool buildSurrogate

  flag specifying whether or not a surrogate is built over the subspace
- int refinementSamples

  Number of refinement samples to use when building a surrogate.
- Iterator fullspaceSampler

  Monte Carlo sampler for the full parameter space.
- IntResponseMap surrResponseMap

  map of responses returned in buildSurrogate mode
- IntIntMap surrIdMap

  map from surrogateModel evaluation ids to RecastModel ids

Static Protected Attributes

- static ActiveSubspaceModel ∗ asmInstance

  static pointer to this class for use in static callbacks

Additional Inherited Members

14.2.1 Detailed Description

Active subspace model for input (variable space) reduction.

Specialization of a RecastModel that identifies an active subspace during build phase and creates a RecastModel in the reduced space

14.2.2 Constructor & Destructor Documentation

14.2.2.1 ActiveSubspaceModel (const Model & *sub_model,* unsigned int *dimension,* const RealMatrix & *rotation_matrix,* short *output_level*)

lightweight constructor

An ActiveSubspaceModel will be built over all functions, without differentiating primary vs. secondary constraints. However the associated RecastModel has to differentiate. Currently identifies subspace for continuous variables only, but carries other active variables along for the ride.

References ActiveSubspaceModel::inactiveBasis, ActiveSubspaceModel::initialize_subspace(), Model::mapping-Initialized, Model::modelId, Model::modelType, SubspaceModel::numFullspaceVars, RecastModel::recast_-model_id(), SubspaceModel::reducedBasis, SubspaceModel::reducedRank, RecastModel::root_model_id(), and SubspaceModel::validate_inputs().

14.2.3 Member Function Documentation

14.2.3.1 void derived_init_communicators (ParLevLIter *pl_iter,* int *max_eval_concurrency,* bool *recurse_flag*) [protected], [virtual]

This specialization is because the model is used in multiple contexts in this iterator, depending on build phase. Note that this overrides the default behavior at Iterator which recurses into any submodels.

Reimplemented from Model.

References ActiveSubspaceModel::fullspaceSampler, Iterator::init_communicators(), Model::init_communicators(), Model::mappingInitialized, SubspaceModel::onlineEvalConcurrency, and RecastModel::subModel.

14.2.3.2 Real build_cv_surrogate (Model & *cv_surr_model,* RealMatrix *training_x,* IntResponseMap *training_y,* RealMatrix *test_x,* IntResponseMap *test_y*) [protected]

Build moving least squares surrogate over candidate active subspace.

Build global moving least squares surrogate model to use in cross validation to estimate active subspace size.

References Response::active_set(), Model::continuous_variables(), Response::copy(), Model::current_response(), Model::evaluate(), Model::numFns, and Model::update_approximation().

Referenced by ActiveSubspaceModel::compute_cross_validation_metric().

14.2.3.3 void build_surrogate ( ) [protected]

Build surrogate over active subspace.

Build surrogate over active subspace: initialize surrogateModel.

References Response::active_set(), Iterator::active_set_request_values(), Iterator::all_responses(), Iterator::all-_samples(), Model::append_approximation(), Model::assign_rep(), Model::current_response(), ActiveSubspace-Model::fullspaceSampler, ActiveSubspaceModel::leftSingularVectors, SubspaceModel::miPLIndex, Model::model-PCIter, Model::outputLevel, SubspaceModel::reducedBasis, SubspaceModel::reducedRank, ActiveSubspace-Model::refinementSamples, Iterator::run(), Iterator::sampling_reference(), Iterator::sampling_reset(), RecastModel-::subModel, and ActiveSubspaceModel::surrogateModel.

Referenced by ActiveSubspaceModel::initialize_subspace().

14.2.3.4 void uncertain_vars_to_subspace ( ) [protected], [virtual]

translate the characterization of uncertain variables in the native_model to the reduced space of the transformed model

Convert the user-specified normal random variables to the appropriate reduced space variables, based on the orthogonal transformation.

TODO: Generalize to convert other random variable types (non-normal)

TODO: The translation of the correlations from full to reduced space is likely wrong for rank correlations; should be correct for covariance.

Reimplemented from SubspaceModel.

References Dakota::abort_handler(), Variables::continuous_variable_types(), Model::continuous_variables(), Model::currentVariables, ActiveSubspaceModel::inactiveBasis, ActiveSubspaceModel::inactiveVars, Subspace-Model::initialize_base_recast(), Model::multivariate_distribution(), Model::mvDist, SubspaceModel::numFullspace-Vars, Model::outputLevel, SubspaceModel::reducedBasis, SubspaceModel::reducedRank, SubspaceModel-::response_mapping(), SubspaceModel::set_mapping(), RecastModel::subModel, SubspaceModel::uncertain_-vars_to_subspace(), and ActiveSubspaceModel::variables_mapping().

14.2.3.5 void variables_mapping (const Variables & *recast_y_vars,* Variables & *sub_model_x_vars*) [static], [protected]

map the active continuous recast variables to the active submodel variables (linear transformation)

Perform the variables mapping from recast reduced dimension variables y to original model x variables via linear transformation. Maps only continuous variables.

References ActiveSubspaceModel::asmInstance, Variables::continuous_variables(), Variables::continuous_-variables_view(), ActiveSubspaceModel::inactiveBasis, ActiveSubspaceModel::inactiveVars, Model::output_level(), and SubspaceModel::reducedBasis.

Referenced by ActiveSubspaceModel::uncertain_vars_to_subspace().

14.2.4 Member Data Documentation

14.2.4.1 ActiveSubspaceModel * asmInstance [static], [protected]

static pointer to this class for use in static callbacks

initialization of static needed by RecastModel callbacks

Referenced by ActiveSubspaceModel::assign_instance(), and ActiveSubspaceModel::variables_mapping().

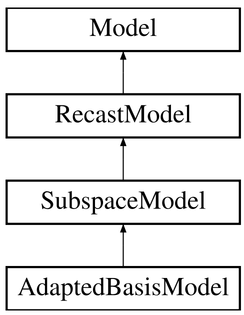
The documentation for this class was generated from the following files:

- ActiveSubspaceModel.hpp
- ActiveSubspaceModel.cpp

14.3 AdaptedBasisModel Class Reference

Adapted basis model for input (variable space) reduction.

Inheritance diagram for AdaptedBasisModel:



Public Member Functions

- AdaptedBasisModel (ProblemDescDB &problem_db)

  Problem database constructor.
- ∼AdaptedBasisModel ()

  destructor

Protected Member Functions

- void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)
- void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)

  portion of set_communicators() specific to derived model classes
- void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag)

  portion of free_communicators() specific to derived model classes
- Model get_sub_model (ProblemDescDB &problem_db)

  retrieve the sub-Model from the DB to pass up the constructor chain
- void compute_subspace ()

  sample the model's gradient, computed the SVD, and form the active subspace rotation matrix.
- void truncate_rotation ()

  use the truncation methods to identify the size of a reduced subspace
- void uncertain_vars_to_subspace ()

translate the characterization of uncertain variables in the native_model to the reduced space of the transformed model

- void validate_inputs ()

  validate the build controls and set defaults

Static Protected Member Functions

- static void variables_mapping (const Variables &recast_xi_vars, Variables &sub_model_x_vars)

  map the active continuous recast variables to the active submodel variables (linear transformation)

Protected Attributes

- short method_rotation

  store the rotation_method input specification, prior to run-time Options right now:
- Real **adaptedBasisTruncationTolerance**
- int **subspaceDimension**
- NonDPolynomialChaos ∗ pcePilotExpRepPtr

  BMA TODO: The initialization order of this Model, base RecastModel, and interdependence with PCE and its sub-model need fixing. Cannot make this a shared_ptr as it'll get default constructed and cleared after get_sub_model is called. Leaving as Iterator∗ for now, but we're just getting lucky with initialization (would probably break in a DEBUG build.
- Iterator pcePilotExpansion

  low-order (linear or quadratic) PCE generator for computing rotation matrices A_i for each of the QoI; this is low-order and potentially high-dimension whereas a client PCE could be high-order in the reduced dimension

Additional Inherited Members

14.3.1 Detailed Description

Adapted basis model for input (variable space) reduction.

Specialization of a RecastModel that creates an adapted basis model during build phase and creates a RecastModel in the reduced space

14.3.2 Member Function Documentation

14.3.2.1 void derived_init_communicators (ParLevLIter *pl_iter,* int *max_eval_concurrency,* bool *recurse_flag*) [protected], [virtual]

This specialization is because the model is used in multiple contexts depending on build phase.

Reimplemented from Model.

References Iterator::init_communicators(), Model::init_communicators(), SubspaceModel::onlineEvalConcurrency, AdaptedBasisModel::pcePilotExpansion, and RecastModel::subModel.

14.3.2.2 void uncertain_vars_to_subspace ( ) [protected], [virtual]

translate the characterization of uncertain variables in the native_model to the reduced space of the transformed model

Define the distribution of recast reduced dimension variables . They are standard Gaussian in adapted basis model.

Reimplemented from SubspaceModel.

References Model::continuous_variable_labels(), Variables::continuous_variable_types(), Model::continuous_variables(), Model::currentVariables, SubspaceModel::initialize_base_recast(), Model::mvDist, Model::outputLevel, SubspaceModel::reducedRank, SubspaceModel::response_mapping(), SubspaceModel::set_mapping(), SubspaceModel::uncertain_vars_to_subspace(), and AdaptedBasisModel::variables_mapping().

14.3.2.3 void variables_mapping (const Variables & *reduced_vars*, Variables & *full_vars*) [static], [protected]

map the active continuous recast variables to the active submodel variables (linear transformation)

Perform the variables mapping from recast reduced dimension variables to original model variables via linear transformation. Maps only continuous variables.

References Variables::continuous_variables(), Variables::continuous_variables_view(), Model::output_level(), SubspaceModel::reduced_basis(), and SubspaceModel::smInstance.

Referenced by AdaptedBasisModel::uncertain_vars_to_subspace().

14.3.3 Member Data Documentation

14.3.3.1 short method_rotation [protected]

store the rotation_method input specification, prior to run-time Options right now:

- linear = use the linear PCE coefficients
- norm = use normalized sensitivity along each direction

Referenced by AdaptedBasisModel::compute_subspace().

14.3.3.2 NonDPolynomialChaos∗ pcePilotExpRepPtr [protected]

BMA TODO: The initialization order of this Model, base RecastModel, and interdependence with PCE and its submodel need fixing. Cannot make this a shared_ptr as it'll get default constructed and cleared after get_sub_model is called. Leaving as Iterator∗ for now, but we're just getting lucky with initialization (would probably break in a DEBUG build.

PCE representation pointer that is initialized in get_sub_model() and then assigned into pcePilotExpansion in the constructor initializer list

Referenced by AdaptedBasisModel::AdaptedBasisModel(), AdaptedBasisModel::compute_subspace(), and AdaptedBasisModel::get_sub_model().

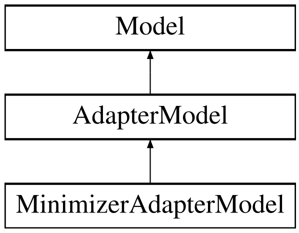
The documentation for this class was generated from the following files:

- AdaptedBasisModel.hpp
- AdaptedBasisModel.cpp

14.4 AdapterModel Class Reference

Derived model class which wraps call-back functions for solving minimization sub-problems.

Inheritance diagram for AdapterModel:



Public Member Functions

- AdapterModel (const Variables &initial_pt, const Constraints &cons, const Response &resp, void(∗resp_map)(const Variables &vars, const ActiveSet &set, Response &response)=NULL)

    standard full constructor with minimizer-specific bounds/targets; doubles as a partial constructor given default value for response mapping function pointer
- AdapterModel (void(∗resp_map)(const Variables &vars, const ActiveSet &set, Response &response))

    alternate partial constructor; constructs response map but requires subsequent init_minimizer_data() call
- ∼AdapterModel ()

    destructor
- void initialize_response_map (void(∗resp_map)(const Variables &vars, const ActiveSet &set, Response &response))

    initialize map callbacks after alternate construction

Protected Member Functions

- void derived_evaluate (const ActiveSet &set)

    portion of evaluate() specific to AdapterModel
- void derived_evaluate_nowait (const ActiveSet &set)

    portion of evaluate_nowait() specific to AdapterModel
- const IntResponseMap & derived_synchronize ()

    portion of synchronize() specific to AdapterModel
- const IntResponseMap & derived_synchronize_nowait ()

    portion of synchronize_nowait() specific to AdapterModel
- int derived_evaluation_id () const

    return the current evaluation id for the AdapterModel

Protected Attributes

- int adapterModelEvalCntr

    local evaluation id counter used for id mapping
- IntVariablesMap adapterVarsMap

    map of variables used by derived_evaluate_nowait(). Caches values needed for evaluation in synchronization routines.
- IntActiveSetMap adapterSetMap

    map of active set passed to derived_evaluate_nowait(). Caches values needed for evaluation in synchronization routines.
- IntResponseMap adapterRespMap

    map of responses returned by derived_synchronize() and derived_synchronize_nowait()

Private Attributes

- void(∗ respMapping)(const Variables &vars, const ActiveSet &set, Response &response)

    holds pointer for primary response mapping function passed in ctor/initialize

Additional Inherited Members

14.4.1 Detailed Description

Derived model class which wraps call-back functions for solving minimization sub-problems.

The AdapterModel class uses C-style function pointers to: (a) allow use of existing Iterator constructor APIs that utilize an incoming Model to extract sub-problem data, and (b) enable Model recursions on top of these call-backs.

14.4.2 Constructor & Destructor Documentation

14.4.2.1 AdapterModel (const Variables & *initial_vars,* const Constraints & *cons,* const Response & *resp,* void(∗)(const Variables &vars, const ActiveSet &set, Response &response) *resp_map* = NULL)

standard full constructor with minimizer-specific bounds/targets; doubles as a partial constructor given default value for response mapping function pointer

This constructor creates a generic stand-alone AdapterModel (not part of a derived constructor chain).

References Variables::active_variables(), Model::currentVariables, Model::modelId, Model::modelType, Model::outputLevel, Constraints::update(), and Model::userDefinedConstraints.

14.4.2.2 AdapterModel (void(∗)(const Variables &vars, const ActiveSet &set, Response &response) *resp_map*)

alternate partial constructor; constructs response map but requires subsequent init_minimizer_data() call

Base portion of derived constructor chains.

References Model::modelType.

14.4.3 Member Function Documentation

14.4.3.1 void derived_evaluate (const ActiveSet & *set*) [protected], [virtual]

portion of evaluate() specific to AdapterModel

The AdapterModel is evaluated by an Iterator for a recast problem formulation. Therefore, the currentVariables, incoming active set, and output currentResponse all correspond to the recast inputs/outputs.

Reimplemented from Model.

References AdapterModel::adapterModelEvalCntr, Model::currentResponse, Model::currentVariables, and AdapterModel::respMapping.

The documentation for this class was generated from the following files:

- AdapterModel.hpp
- AdapterModel.cpp

14.5 AddAttributeVisitor Class Reference

Objects of this class are called by boost::appy_visitor to add attributes to HDF5 objects.

Inherits static_visitor<>.

Public Member Functions

- AddAttributeVisitor (const String &location, const std::shared_ptr< HDF5IOHelper > &hdf5_stream)

The attributes will be added to the HDF5 object at location, using the HDF5IOHelper instance hdf5_stream.

- template<typename T >
  void operator() (const ResultAttribute< T > &a) const

  Called by boost::apply_vistitor to process a ResultAttribute.

Private Attributes

- String location

  Link name of the HDF5 object to add attributes to.
- std::shared_ptr< HDF5IOHelper > hdf5Stream

  HDF5IOHelper instance.

14.5.1 Detailed Description

Objects of this class are called by boost::appy_visitor to add attributes to HDF5 objects.

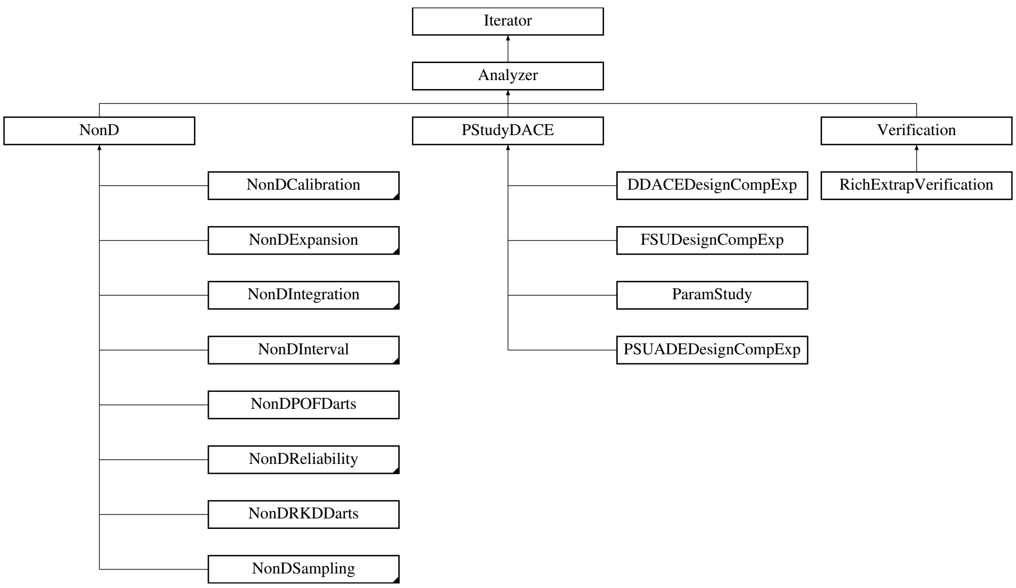
The documentation for this class was generated from the following file:

- ResultsDBHDF5.hpp

14.6 Analyzer Class Reference

Base class for NonD, DACE, and ParamStudy branches of the iterator hierarchy.

Inheritance diagram for Analyzer:



Public Member Functions

- const VariablesArray & all_variables ()

  return the complete set of evaluated variables
- const RealMatrix & all_samples ()

  return the complete set of evaluated samples
- const IntResponseMap & all_responses () const

return the complete set of computed responses
- bool resize ()

  reinitializes iterator based on new variable size
- size_t num_samples () const
- virtual void vary_pattern (bool pattern_flag)

  sets varyPattern in derived classes that support it

Protected Member Functions

- Analyzer ()

  default constructor
- Analyzer (ProblemDescDB &problem_db, Model &model)

  standard constructor
- Analyzer (unsigned short method_name, Model &model)

  alternate constructor for instantiations "on the fly" with a Model
- Analyzer (unsigned short method_name)

  alternate constructor for instantiations "on the fly" without a Model
- ∼Analyzer ()

  destructor
- virtual void get_parameter_sets (Model &model)

  Generate one block of numSamples samples (ndim ∗ num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.
- virtual void get_parameter_sets (Model &model, const size_t num_samples, RealMatrix &design_matrix)

  Generate one block of numSamples samples (ndim ∗ num_samples), populating design_matrix.
- virtual void update_model_from_sample (Model &model, const Real ∗sample_vars)

  update model's current variables with data from sample
- virtual void update_model_from_variables (Model &model, const Variables &vars)

  update model's current variables with data from vars
- virtual void sample_to_variables (const Real ∗sample_vars, Variables &vars)

  convert column of samples array to variables; derived classes may reimplement for more than active continuous variables
- void update_from_model (const Model &model)

  set inherited data attributes based on extractions from incoming model
- void initialize_run ()

  utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
- void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void post_run (std::ostream &s)

  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- void finalize_run ()

  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
- void pre_output ()
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final iterator results
- const Model & algorithm_space_model () const
- const Variables & variables_results () const

  return a single final iterator solution (variables)
- const Response & response_results () const

  return a single final iterator solution (response)

- const VariablesArray & variables_array_results ()

  return multiple final iterator solutions (variables). This should only be used if returns_multiple_points() returns true.
- const ResponseArray & response_array_results ()

  return multiple final iterator solutions (response). This should only be used if returns_multiple_points() returns true.
- void response_results_active_set (const ActiveSet &set)

  set the requested data for the final iterator response results
- bool compact_mode () const

  returns Analyzer::compactMode
- bool returns_multiple_points () const

  indicates if this iterator returns multiple final points. Default return is false. Override to return true if appropriate.
- void evaluate_parameter_sets (Model &model, bool log_resp_flag, bool log_best_flag)

  perform function evaluations to map parameter sets (allVariables) into response sets (allResponses)
- void get_vbd_parameter_sets (Model &model, size_t num_samples)

  generate replicate parameter sets for use in variance-based decomposition
- void compute_vbd_stats (const size_t num_samples, const IntResponseMap &resp_samples)

  compute VBD-based Sobol indices
- void archive_sobol_indices () const

  archive VBD-based Sobol indices
- virtual void archive_model_variables (const Model &, size_t idx) const

  archive model evaluation points
- virtual void archive_model_response (const Response &, size_t idx) const

  archive model evaluation responses
- void read_variables_responses (int num_evals, size_t num_vars)

  convenience function for reading variables/responses (used in derived classes post_input)
- void print_sobol_indices (std::ostream &s) const

  Printing of VBD results.
- void samples_to_variables_array (const RealMatrix &sample_matrix, VariablesArray &vars_array)

  convert samples array to variables array; e.g., allSamples to allVariables
- virtual void variables_to_sample (const Variables &vars, Real *sample_c_vars)

  convert the active continuous variables into a column of allSamples
- void variables_array_to_samples (const VariablesArray &vars_array, RealMatrix &sample_matrix)

  convert variables array to samples array; e.g., allVariables to allSamples

Protected Attributes

- size_t numFunctions

  number of response functions
- size_t numContinuousVars

  number of active continuous vars
- size_t numDiscreteIntVars

  number of active discrete integer vars
- size_t numDiscreteStringVars

  number of active discrete string vars
- size_t numDiscreteRealVars

  number of active discrete real vars
- bool compactMode

  switch for allSamples (compact mode) instead of allVariables (normal mode)
- VariablesArray allVariables

  array of all variables to be evaluated in evaluate_parameter_sets()
- RealMatrix allSamples

compact alternative to allVariables

- IntResponseMap allResponses

  array of all responses to be computed in evaluate_parameter_sets()
- StringArray allHeaders

  array of headers to insert into output while evaluating allVariables
- size_t numObjFns

  number of objective functions
- size_t numLSqTerms

  number of least squares terms
- RealPairPRPMultiMap bestVarsRespMap

  map which stores best set of solutions

Private Member Functions

- void compute_best_metrics (const Response &response, std::pair< Real, Real > &metrics)

  compares current evaluation to best evaluation and updates best
- void update_best (const Variables &vars, int eval_id, const Response &response)

  compares current evaluation to best evaluation and updates best
- void update_best (const Real ∗sample_c_vars, int eval_id, const Response &response)

  compares current evaluation to best evaluation and updates best

Private Attributes

- int writePrecision

  write precision as specified by the user
- Real vbdDropTol

  tolerance for omitting output of small VBD indices
- RealVectorArray S4

  VBD main effect indices.
- RealVectorArray T4

  VBD total effect indices.

Additional Inherited Members

14.6.1 Detailed Description

Base class for NonD, DACE, and ParamStudy branches of the iterator hierarchy.

The Analyzer class provides common data and functionality for various types of systems analysis, including nondeterministic analysis, design of experiments, and parameter studies.

14.6.2 Member Function Documentation

14.6.2.1 size_t num_samples ( ) const [inline], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Iterator.

Reimplemented in NonDSampling, NonDQuadrature, NonDSparseGrid, NonDCubature, DDACEDesignCompExp, FSUDesignCompExp, and PSUADEDesignCompExp.

References Model::derivative_concurrency(), Iterator::iteratedModel, and Iterator::maxEvalConcurrency.

Referenced by NonDDREAMBayesCalibration::archive_acceptance_chain(), NonDDREAMBayesCalibration::cache_chain(), NonDBayesCalibration::compute_statistics(), Analyzer::compute_vbd_stats(), NonDGlobalReliability::get_best_sample(), Analyzer::get_vbd_parameter_sets(), NonDPolynomialChaos::ratio_samples_to_order(), Analyzer::samples_to_variables_array(), and Analyzer::variables_array_to_samples().

14.6.2.2 void sample_to_variables (const Real * *sample_c_vars,* Variables & *vars*) [protected], [virtual]

convert column of samples array to variables; derived classes may reimplement for more than active continuous variables

Default mapping that maps into continuous part of Variables only

Reimplemented in NonDSampling.

References Variables::adiv(), Variables::adrv(), Variables::all_discrete_int_variables(), Variables::all_discrete_real_variables(), Variables::continuous_variable(), Model::current_variables(), Variables::inactive_continuous_variables(), Variables::is_null(), Iterator::iteratedModel, Analyzer::numContinuousVars, and Variables::shared_data().

Referenced by NonDLHSEvidence::post_process_samples(), Analyzer::pre_output(), Analyzer::samples_to_variables_array(), and Analyzer::update_best().

14.6.2.3 void initialize_run ( ) [protected], [virtual]

utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers

Perform initialization phases of run sequence, like allocating memory and setting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's initialize_run(), typically *before* performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in NonD.

References Model::initialize_mapping(), Model::is_null(), Iterator::iteratedModel, Iterator::methodPCIter, Analyzer::resize(), Model::set_evaluation_reference(), and Iterator::summaryOutputFlag.

Referenced by NonD::initialize_run().

14.6.2.4 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in NonDSampling, NonDBayesCalibration, NonDLHSSampling, NonDLocalReliability, NonDNonHierarchSampling, DDACEDesignCompExp, NonDRKDDarts, NonDEnsembleSampling, FSUDesignCompExp, ParamStudy, PSUADEDesignCompExp, NonDGlobalReliability, and NonDMultilevControlVarSampling.

References Analyzer::bestVarsRespMap.

Referenced by NonDGlobalReliability::pre_run(), PSUADEDesignCompExp::pre_run(), ParamStudy::pre_run(), FSUDesignCompExp::pre_run(), NonDRKDDarts::pre_run(), DDACEDesignCompExp::pre_run(), NonDLocalReliability::pre_run(), NonDBayesCalibration::pre_run(), and NonDSampling::pre_run().

14.6.2.5 void post_run (std::ostream & *s*) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in NonDRKDDarts, NonDLHSSampling, DDACEDesignCompExp, NonDEnsembleSampling, FS-UDesignCompExp, NonDReliability, ParamStudy, and PSUADEDesignCompExp.

References Model::is_null(), Iterator::iteratedModel, Model::print_evaluation_summary(), Analyzer::print_results(), and Iterator::summaryOutputFlag.

Referenced by PSUADEDesignCompExp::post_run(), NonDReliability::post_run(), ParamStudy::post_run(), FSU-DesignCompExp::post_run(), NonDEnsembleSampling::post_run(), DDACEDesignCompExp::post_run(), NonDL-HSSampling::post_run(), and NonDRKDDarts::post_run().

14.6.2.6 void finalize_run ( ) [protected], [virtual]

utility function to perform common operations following post_run(); deallocation and resetting of instance pointers

Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's finalize_run(), typically *after* performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in NonD.

References Model::finalize_mapping(), Model::is_null(), Iterator::iteratedModel, and Analyzer::resize().

Referenced by NonD::finalize_run().

14.6.2.7 void pre_output ( ) [protected], [virtual]

Generate tabular output with active variables (compactMode) or all variables with their labels and response labels, with no data. Variables are sequenced {cv, div, drv}

Reimplemented from Iterator.

References Analyzer::allSamples, Analyzer::allVariables, ParallelLibrary::command_line_pre_run_output(), ParallelLibrary::command_line_user_modes(), Analyzer::compactMode, Variables::copy(), Model::current_-response(), Model::current_variables(), Model::interface_id(), Iterator::iteratedModel, Iterator::outputLevel, Iterator-::parallelLib, ProgramOptions::pre_run_output_format(), ParallelLibrary::program_options(), Analyzer::sample_to_-variables(), Dakota::write_precision, Variables::write_tabular(), and Analyzer::writePrecision.

14.6.2.8 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Iterator.

Reimplemented in NonDPolynomialChaos, NonDGPMSABayesCalibration, NonDLHSSampling, NonDMultilevel-PolynomialChaos, NonDBayesCalibration, NonDMultilevelFunctionTrain, NonDPOFDarts, NonDQUESOBayes-Calibration, NonDMultilevelStochCollocation, NonDAdaptImpSampling, NonDLocalReliability, NonDWASABI-BayesCalibration, NonDAdaptiveSampling, NonDExpansion, NonDGPImpSampling, NonDMUQBayesCalibration, NonDEnsembleSampling, NonDInterval, PStudyDACE, NonDGlobalReliability, Verification, and RichExtrapVerification.

References Analyzer::bestVarsRespMap, ParamResponsePair::eval_id(), Response::function_values(), Analyzer::numLSqTerms, Analyzer::numObjFns, ParamResponsePair::response(), and ParamResponsePair::variables().

Referenced by Analyzer::post_run(), Verification::print_results(), PStudyDACE::print_results(), and NonDLHSSampling::print_results().

14.6.2.9 const Model & algorithm_space_model ( ) const [inline], [protected], [virtual]

default definition that gets redefined in selected derived Minimizers

Reimplemented from Iterator.

Reimplemented in NonDBayesCalibration, NonDExpansion, NonDReliability, and NonDGlobalInterval.

References Iterator::iteratedModel.

14.6.2.10 void evaluate_parameter_sets (Model & *model,* bool *log_resp_flag,* bool *log_best_flag*) [protected]

perform function evaluations to map parameter sets (allVariables) into response sets (allResponses)

Convenience function for derived classes with sets of function evaluations to perform (e.g., NonDSampling, DDACEDesignCompExp, FSUDesignCompExp, ParamStudy).

References ResultsManager::active(), Iterator::activeSet, Analyzer::allHeaders, Analyzer::allResponses, Analyzer::allSamples, Analyzer::allVariables, Analyzer::archive_model_response(), Analyzer::archive_model_variables(), Model::asynch_flag(), Analyzer::compactMode, Response::copy(), Model::current_response(), Model::current_variables(), Model::evaluate(), Model::evaluate_nowait(), Model::evaluation_id(), Iterator::resultsDB, Model::synchronize(), Analyzer::update_best(), Analyzer::update_model_from_sample(), and Analyzer::update_model_from_variables().

Referenced by ParamStudy::core_run(), PSUADEDesignCompExp::core_run(), FSUDesignCompExp::core_run(), DDACEDesignCompExp::core_run(), NonDAdaptImpSampling::core_run(), NonDLHSSampling::core_run(), NonDIntegration::core_run(), NonDSampling::core_run(), NonDSparseGrid::evaluate_grid_increment(), NonDQuadrature::evaluate_grid_increment(), NonDMultilevelSampling::evaluate_ml_sample_increment(), NonDMultilevControlVarSampling::evaluate_pilot(), NonDSparseGrid::evaluate_set(), NonDControlVariateSampling::lf_increment(), NonDMultilevControlVarSampling::multilevel_control_variate_mc_offline_pilot(), NonDMultilevControlVarSampling::multilevel_control_variate_mc_Qcorr(), NonDControlVariateSampling::shared_increment(), and NonDBayesCalibration::update_model().

14.6.2.11 void get_vbd_parameter_sets (Model & *model,* size_t *num_samples*) [protected]

generate replicate parameter sets for use in variance-based decomposition

Generate (numvars + 2)∗num_samples replicate sets for VBD, populating allSamples(numvars, (numvars + 2)∗num_samples)

References Dakota::abort_handler(), Analyzer::allSamples, Analyzer::compactMode, Analyzer::get_parameter_sets(), Analyzer::num_samples(), Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, and Analyzer::vary_pattern().

Referenced by FSUDesignCompExp::pre_run(), DDACEDesignCompExp::pre_run(), and NonDLHSSampling::pre_run().

14.6.2.12 void compute_vbd_stats (const size_t *num_samples,* const IntResponseMap & *resp_samples*) [protected]

compute VBD-based Sobol indices

Calculation of sensitivity indices obtained by variance based decomposition. These indices are obtained by the

Saltelli version of the Sobol VBD which uses (K+2)*N function evaluations, where K is the number of dimensions (uncertain vars) and N is the number of samples.

References Dakota::abort_handler(), Analyzer::allSamples, Analyzer::num_samples(), Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, Analyzer::numFunctions, Analyzer::S4, and Analyzer::T4.

Referenced by FSUDesignCompExp::post_run(), DDACEDesignCompExp::post_run(), and NonDLHSSampling::post_run().

14.6.2.13 void archive_sobol_indices ( ) const [protected]

archive VBD-based Sobol indices

printing of variance based decomposition indices.

References ResultsManager::active(), Model::continuous_variable_labels(), Model::discrete_int_variable_labels(), Model::discrete_real_variable_labels(), ResultsManager::insert(), Iterator::iteratedModel, main(), Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numFunctions, Model::response_labels(), Iterator::resultsDB, Iterator::run_identifier(), Analyzer::S4, Analyzer::T4, and Analyzer::vbdDropTol.

Referenced by NonDLHSSampling::post_run().

14.6.2.14 void read_variables_responses (int *num_evals*, size_t *num_vars*) [protected]

convenience function for reading variables/responses (used in derived classes post_input)

read num_evals variables/responses from file

References Dakota::abort_handler(), Analyzer::allResponses, Analyzer::allSamples, Analyzer::allVariables, ParallelLibrary::command_line_post_run_input(), ParallelLibrary::command_line_user_modes(), Analyzer::compactMode, Response::copy(), Variables::copy(), Model::current_response(), Model::current_variables(), Dakota::data_pairs, ParamResponsePair::eval_id(), Model::evaluation_cache(), Iterator::iteratedModel, Model::manage_data_recastings(), Analyzer::numLSqTerms, Analyzer::numObjFns, Iterator::outputLevel, Iterator::parallelLib, ProgramOptions::post_run_input_format(), ParallelLibrary::program_options(), ParamResponsePair::response(), Model::restart_file(), Analyzer::update_best(), Model::user_space_to_iterator_space(), ParamResponsePair::variables(), Analyzer::variables_to_sample(), and ParallelLibrary::write_restart().

Referenced by PSUADEDesignCompExp::post_input(), ParamStudy::post_input(), FSUDesignCompExp::post_input(), DDACEDesignCompExp::post_input(), and NonDLHSSampling::post_input().

14.6.2.15 void print_sobol_indices (std::ostream & *s*) const [protected]

Printing of VBD results.

printing of variance based decomposition indices.

References Model::continuous_variable_labels(), Model::discrete_int_variable_labels(), Model::discrete_real_variable_labels(), Iterator::iteratedModel, main(), Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numFunctions, Model::response_labels(), Analyzer::S4, Analyzer::T4, Analyzer::vbdDropTol, and Dakota::write_precision.

Referenced by PStudyDACE::print_results(), and NonDLHSSampling::print_results().

14.6.2.16 void variables_to_sample (const Variables & *vars*, Real * *sample_c_vars*) [protected], [virtual]

convert the active continuous variables into a column of allSamples

Default implementation maps active continuous variables only

Reimplemented in NonDSampling.

References Variables::continuous_variables(), and Analyzer::numContinuousVars.

Referenced by Analyzer::read_variables_responses(), and Analyzer::variables_array_to_samples().

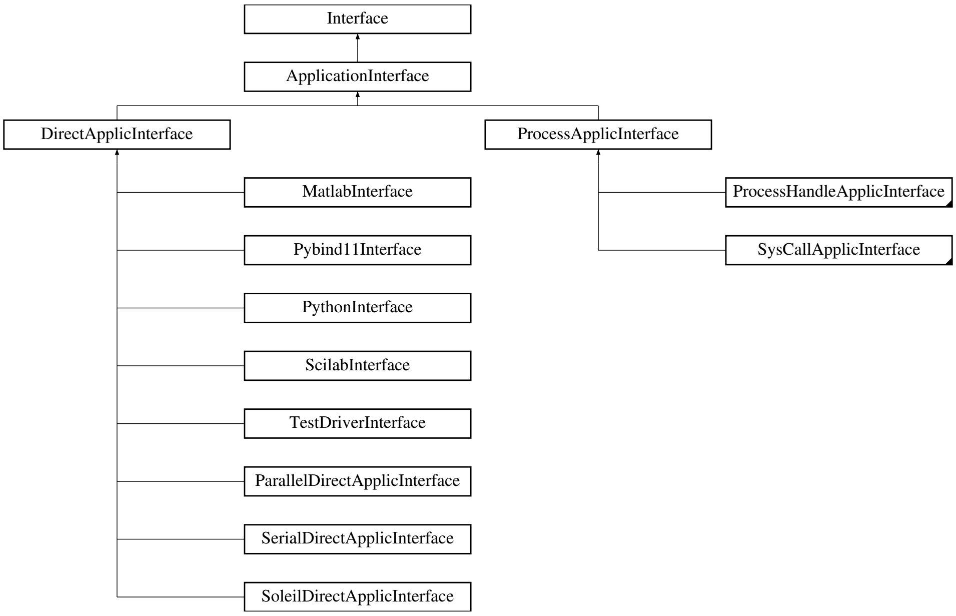
The documentation for this class was generated from the following files:

- DakotaAnalyzer.hpp
- DakotaAnalyzer.cpp

14.7 ApplicationInterface Class Reference

Derived class within the interface class hierarchy for supporting interfaces to simulation codes.

Inheritance diagram for ApplicationInterface:



Public Member Functions

- ApplicationInterface (const ProblemDescDB &problem_db)

  constructor
- ∼ApplicationInterface ()

  destructor

Protected Member Functions

- void init_communicators (const IntArray &message_lengths, int max_eval_concurrency)

  allocate communicator partitions for concurrent evaluations within an iterator and concurrent multiprocessor analyses within an evaluation.
- void set_communicators (const IntArray &message_lengths, int max_eval_concurrency)

  set the local parallel partition data for an interface (the partitions are already allocated in ParallelLibrary).
- void init_serial ()
- int asynch_local_evaluation_concurrency () const

  return asynchLocalEvalConcurrency
- short interface_synchronization () const

  return interfaceSynchronization

- bool evaluation_cache () const

  return evalCacheFlag
- bool restart_file () const

  return evalCacheFlag
- String final_eval_id_tag (int fn_eval_id)

  form and return the final evaluation ID tag, appending iface ID if needed
- void map (const Variables &vars, const ActiveSet &set, Response &response, bool asynch_flag=false)

  Provides a "mapping" of variables to responses using a simulation. Protected due to Interface letter-envelope idiom.
- void manage_failure (const Variables &vars, const ActiveSet &set, Response &response, int failed_eval_id)

  manages a simulation failure using abort/retry/recover/continuation
- const IntResponseMap & synchronize ()

  executes a blocking schedule for asynchronous evaluations in the beforeSynchCorePRPQueue and returns all jobs
- const IntResponseMap & synchronize_nowait ()

  executes a nonblocking schedule for asynchronous evaluations in the beforeSynchCorePRPQueue and returns a partial set of completed jobs
- void serve_evaluations ()

  run on evaluation servers to serve the iterator master
- void stop_evaluation_servers ()

  used by the iterator master to terminate evaluation servers
- bool check_multiprocessor_analysis (bool warn)

  checks on multiprocessor analysis configuration
- bool check_asynchronous (bool warn, int max_eval_concurrency)

  checks on asynchronous configuration (for direct interfaces)
- bool check_multiprocessor_asynchronous (bool warn, int max_eval_concurrency)

  checks on asynchronous settings for multiprocessor partitions
- String final_batch_id_tag ()

  form and return the final batch ID tag
- virtual void derived_map (const Variables &vars, const ActiveSet &set, Response &response, int fn_eval_id)

  Called by map() and other functions to execute the simulation in synchronous mode. The portion of performing an evaluation that is specific to a derived class.
- virtual void derived_map_asynch (const ParamResponsePair &pair)

  Called by map() and other functions to execute the simulation in asynchronous mode. The portion of performing an asynchronous evaluation that is specific to a derived class.
- virtual void wait_local_evaluations (PRPQueue &prp_queue)

  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version waits for at least one completion.
- virtual void test_local_evaluations (PRPQueue &prp_queue)

  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version is nonblocking and will return without any completions if none are immediately available.
- virtual void init_communicators_checks (int max_eval_concurrency)

  perform construct-time error checks on the parallel configuration
- virtual void set_communicators_checks (int max_eval_concurrency)

  perform run-time error checks on the parallel configuration
- void master_dynamic_schedule_analyses ()

  blocking dynamic schedule of all analyses within a function evaluation using message passing
- void serve_analyses_synch ()

  serve the master analysis scheduler and manage one synchronous analysis job at a time
- virtual int synchronous_local_analysis (int analysis_id)

  Execute a particular analysis (identified by analysis_id) synchronously on the local processor. Used for the derived class specifics within ApplicationInterface::serve_analyses_synch().

Protected Attributes

- ParallelLibrary & parallelLib

    reference to the ParallelLibrary object used to manage MPI partitions for the concurrent evaluations and concurrent analyses parallelism levels
- bool batchEval

    flag indicating usage of batch evaluation facilities, where a set of jobs is launched and scheduled as a unit rather than individually
- bool asynchFlag

    flag indicating usage of asynchronous evaluation
- int batchIdCntr

    maintain a count of the batches
- bool suppressOutput

    flag for suppressing output on slave processors
- int evalCommSize

    size of evalComm
- int evalCommRank

    processor rank within evalComm
- int evalServerId

    evaluation server identifier
- bool eaDedMasterFlag

    flag for dedicated master partitioning at ea level
- int analysisCommSize

    size of analysisComm
- int analysisCommRank

    processor rank within analysisComm
- int analysisServerId

    analysis server identifier
- int numAnalysisServers

    current number of analysis servers
- bool multiProcAnalysisFlag

    flag for multiprocessor analysis partitions
- bool asynchLocalAnalysisFlag

    flag for asynchronous local parallelism of analyses
- int asynchLocalAnalysisConcurrency

    limits the number of concurrent analyses in asynchronous local scheduling and specifies hybrid concurrency when message passing
- int asynchLocalEvalConcSpec

    user specification for asynchronous local evaluation concurrency
- int asynchLocalAnalysisConcSpec

    user specification for asynchronous local analysis concurrency
- int numAnalysisDrivers

    the number of analysis drivers used for each function evaluation (from the analysis_drivers interface specification)
- IntSet completionSet

    the set of completed fn_eval_id's populated by wait_local_evaluations() and test_local_evaluations()
- String failureMessage

    base message for managing failed evals; will be followed with more details in screen output

Private Member Functions

- bool duplication_detect (const Variables &vars, Response &response, bool asynch_flag)

    checks data_pairs and beforeSynchCorePRPQueue to see if the current evaluation request has already been performed or queued
- void init_default_asv (size_t num_fns)

    initialize default ASV if needed; this is done at run time due to post-construct time Response size changes.
- void master_dynamic_schedule_evaluations ()

    blocking dynamic schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a dedicated master partition; executes on iteratorComm master
- void peer_static_schedule_evaluations ()

    blocking static schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a peer partition; executes on iteratorComm master
- void peer_dynamic_schedule_evaluations ()

    blocking dynamic schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a peer partition; executes on iteratorComm master
- void asynchronous_local_evaluations (PRPQueue &prp_queue)

    perform all jobs in prp_queue using asynchronous approaches on the local processor
- void synchronous_local_evaluations (PRPQueue &prp_queue)

    perform all jobs in prp_queue using synchronous approaches on the local processor
- void master_dynamic_schedule_evaluations_nowait ()

    execute a nonblocking dynamic schedule in a master-slave partition
- void peer_static_schedule_evaluations_nowait ()

    execute a nonblocking static schedule in a peer partition
- void peer_dynamic_schedule_evaluations_nowait ()

    execute a nonblocking dynamic schedule in a peer partition
- void asynchronous_local_evaluations_nowait (PRPQueue &prp_queue)

    launch new jobs in prp_queue asynchronously (if capacity is available), perform nonblocking query of all running jobs, and process any completed jobs (handles both local master- and local peer-scheduling cases)
- void broadcast_evaluation (const ParamResponsePair &pair)

    convenience function for broadcasting an evaluation over an evalComm
- void broadcast_evaluation (int fn_eval_id, const Variables &vars, const ActiveSet &set)

    convenience function for broadcasting an evaluation over an evalComm
- void send_evaluation (PRPQueueIter &prp_it, size_t buff_index, int server_id, bool peer_flag)

    helper function for sending sendBuffers[buff_index] to server
- void receive_evaluation (PRPQueueIter &prp_it, size_t buff_index, int server_id, bool peer_flag)

    helper function for processing recvBuffers[buff_index] within scheduler
- void launch_asynch_local (PRPQueueIter &prp_it)

    launch an asynchronous local evaluation from a queue iterator
- void launch_asynch_local (MPIUnpackBuffer &recv_buffer, int fn_eval_id)

    launch an asynchronous local evaluation from a receive buffer
- void process_asynch_local (int fn_eval_id)

    process a completed asynchronous local evaluation
- void process_synch_local (PRPQueueIter &prp_it)

    process a completed synchronous local evaluation
- void assign_asynch_local_queue (PRPQueue &local_prp_queue, PRPQueueIter &local_prp_iter)

    helper function for creating an initial active local queue by launching asynch local jobs from local_prp_queue, as limited by server capacity
- void assign_asynch_local_queue_nowait (PRPQueue &local_prp_queue, PRPQueueIter &local_prp_iter)

    helper function for updating an active local queue by backfilling asynch local jobs from local_prp_queue, as limited by server capacity
- size_t test_local_backfill (PRPQueue &assign_queue, PRPQueueIter &assign_iter)

helper function for testing active asynch local jobs and then backfilling

- size_t test_receives_backfill (PRPQueueIter &assign_iter, bool peer_flag)

  helper function for testing receive requests and then backfilling jobs

- void serve_evaluations_synch ()

  serve the evaluation message passing schedulers and perform one synchronous evaluation at a time

- void serve_evaluations_synch_peer ()

  serve the evaluation message passing schedulers and perform one synchronous evaluation at a time as part of the 1st peer

- void serve_evaluations_asynch ()

  serve the evaluation message passing schedulers and manage multiple asynchronous evaluations

- void serve_evaluations_asynch_peer ()

  serve the evaluation message passing schedulers and perform multiple asynchronous evaluations as part of the 1st peer

- void set_evaluation_communicators (const IntArray &message_lengths)

  convenience function for updating the local evaluation partition data following ParallelLibrary::init_evaluation_-communicators().

- void set_analysis_communicators ()

  convenience function for updating the local analysis partition data following ParallelLibrary::init_analysis_-communicators().

- void init_serial_evaluations ()

  set concurrent evaluation configuration for serial operations

- void init_serial_analyses ()

  set concurrent analysis configuration for serial operations (e.g., for local executions on a dedicated master)

- const ParamResponsePair & get_source_pair (const Variables &target_vars)

  convenience function for the continuation approach in manage_failure() for finding the nearest successful "source" evaluation to the failed "target"

- void continuation (const Variables &target_vars, const ActiveSet &set, Response &response, const Param-ResponsePair &source_pair, int failed_eval_id)

  performs a 0th order continuation method to step from a successful "source" evaluation to the failed "target". Invoked by manage_failure() for failAction == "continuation".

- void common_input_filtering (const Variables &vars)

  common input filtering operations, e.g. mesh movement

- void common_output_filtering (Response &response)

  common output filtering operations, e.g. data filtering

Private Attributes

- int worldSize

  size of MPI_COMM_WORLD

- int worldRank

  processor rank within MPI_COMM_WORLD

- int iteratorCommSize

  size of iteratorComm

- int iteratorCommRank

  processor rank within iteratorComm

- bool ieMessagePass

  flag for message passing at ie scheduling level

- int numEvalServers

  current number of evaluation servers

- int numEvalServersSpec

  user specification for number of evaluation servers

- int procsPerEvalSpec

user specification for processors per analysis servers

- bool eaMessagePass

    flag for message passing at ea scheduling level

- int numAnalysisServersSpec

    user spec for number of analysis servers

- int procsPerAnalysisSpec

    user specification for processors per analysis servers

- int lenVarsMessage

    length of a MPIPackBuffer containing a Variables object; computed in Model::init_communicators()

- int lenVarsActSetMessage

    length of a MPIPackBuffer containing a Variables object and an ActiveSet object; computed in Model::init_-communicators()

- int lenResponseMessage

    length of a MPIPackBuffer containing a Response object; computed in Model::init_communicators()

- int lenPRPairMessage

    length of a MPIPackBuffer containing a ParamResponsePair object; computed in Model::init_communicators()

- short evalScheduling

    user specification of evaluation scheduling algorithm: {DEFAULT,MASTER,PEER_DYNAMIC,PEER_STATIC}_SCH-EDULING. Used for manual overrides of auto-configure logic in ParallelLibrary::resolve_inputs().

- short analysisScheduling

    user specification of analysis scheduling algorithm: {DEFAULT,MASTER,PEER}_SCHEDULING. Used for manual overrides of the auto-configure logic in ParallelLibrary::resolve_inputs().

- int asynchLocalEvalConcurrency

    limits the number of concurrent evaluations in asynchronous local scheduling and specifies hybrid concurrency when message passing

- bool asynchLocalEvalStatic

    whether the asynchronous local evaluations are to be performed with a static schedule (default false)

- BitArray localServerAssigned

    array with one bit per logical "server" indicating whether a job is currently running on the server (used for asynch local static schedules)

- short interfaceSynchronization

    interface synchronization specification: synchronous (default) or asynchronous

- bool headerFlag

    used by synchronize_nowait to manage header output frequency (since this function may be called many times prior to any completions)

- bool asvControlFlag

    used to manage a user request to deactivate the active set vector control. true = modify the ASV each evaluation as appropriate (default); false = ASV values are static so that the user need not check them on each evaluation.

- bool evalCacheFlag

    used to manage a user request to deactivate the function evaluation cache (i.e., queries and insertions using the data_pairs cache).

- bool nearbyDuplicateDetect

    flag indicating optional usage of tolerance-based duplication detection (less efficient, but helpful when experiencing restart cache misses)

- Real nearbyTolerance

    tolerance value for tolerance-based duplication detection

- bool restartFileFlag

    used to manage a user request to deactivate the restart file (i.e., insertions into write_restart).

- SharedResponseData sharedRespData

    SharedResponseData of associated Response.

- String gradientType

    type of gradients present in associated Response

- String hessianType

type of Hessians present in associated Response

- IntSet gradMixedAnalyticIds

  IDs of analytic gradients when mixed gradients present.

- IntSet hessMixedAnalyticIds

  IDs of analytic gradients when mixed gradients present.

- ShortArray defaultASV

  the static ASV values used when the user has selected asvControl = off

- String failAction

  mitigation action for captured simulation failures: abort, retry, recover, or continuation

- int failRetryLimit

  limit on the number of retries for the retry failAction

- RealVector failRecoveryFnVals

  the dummy function values used for the recover failAction

- IntResponseMap historyDuplicateMap

  used to bookkeep asynchronous evaluations which duplicate data_pairs evaluations. Map key is evalIdCntr, map value is corresponding response.

- std::map< int, std::pair
  < PRPQueueHIter, Response > > beforeSynchDuplicateMap

  used to bookkeep evalIdCntr, beforeSynchCorePRPQueue iterator, and response of asynchronous evaluations which duplicate queued beforeSynchCorePRPQueue evaluations

- PRPQueue beforeSynchCorePRPQueue

  used to bookkeep vars/set/response of nonduplicate asynchronous core evaluations. This is the queue of jobs populated by asynchronous map() that is later scheduled in synchronize() or synchronize_nowait().

- PRPQueue beforeSynchAlgPRPQueue

  used to bookkeep vars/set/response of asynchronous algebraic evaluations. This is the queue of algebraic jobs populated by asynchronous map() that is later evaluated in synchronize() or synchronize_nowait().

- PRPQueue asynchLocalActivePRPQueue

  used by nonblocking asynchronous local schedulers to bookkeep active local jobs

- std::map< int, IntSizetPair > msgPassRunningMap

  used by nonblocking message passing schedulers to bookkeep which jobs are running remotely

- int nowaitEvalIdRef

  fnEvalId reference point for preserving modulo arithmetic-based job assignment in case of peer static nonblocking schedulers

- MPIPackBuffer * sendBuffers

  array of pack buffers for evaluation jobs queued to a server

- MPIUnpackBuffer * recvBuffers

  array of unpack buffers for evaluation jobs returned by a server

- MPI_Request * recvRequests

  array of requests for nonblocking evaluation receives

14.7.1 Detailed Description

Derived class within the interface class hierarchy for supporting interfaces to simulation codes.

ApplicationInterface provides an interface class for performing parameter to response mappings using simulation code(s). It provides common functionality for a number of derived classes and contains the majority of all of the scheduling algorithms in DAKOTA. The derived classes provide the specifics for managing code invocations using system calls, forks, direct procedure calls, or distributed resource facilities.

14.7.2 Member Function Documentation

14.7.2.1 void init_serial ( ) [inline], [protected], [virtual]

DataInterface.cpp defaults of 0 servers are needed to distinguish an explicit user request for 1 server (serialization of a parallelism level) from no user request (use parallel auto-config). This default causes problems when init_communicators() is not called for an interface object (e.g., static scheduling fails in DirectApplicInterface::derived_map() for NestedModel::optionalInterface). This is the reason for this function: to reset certain defaults for interface objects that are used serially.

Reimplemented from Interface.

References ApplicationInterface::init_serial_analyses(), and ApplicationInterface::init_serial_evaluations().

14.7.2.2 void map (const Variables & *vars*, const ActiveSet & *set*, Response & *response*, bool *asynch_flag* = false) [protected], [virtual]

Provides a "mapping" of variables to responses using a simulation. Protected due to Interface letter-envelope idiom.

The function evaluator for application interfaces. Called from derived_evaluate() and derived_evaluate_nowait() in derived Model classes. If asynch_flag is not set, perform a blocking evaluation (using derived_map()). If asynch_flag is set, add the job to the beforeSynchCorePRPQueue queue for execution by one of the scheduler routines in synchronize() or synchronize_nowait(). Duplicate function evaluations are detected with duplication_detect().

Reimplemented from Interface.

References Response::active_set(), Interface::algebraic_mappings(), Interface::algebraicMappings, Interface::asv_mapping(), ApplicationInterface::asvControlFlag, ApplicationInterface::batchEval, ApplicationInterface::beforeSynchAlgPRPQueue, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::broadcast_evaluation(), Response::copy(), Interface::coreMappings, Interface::currEvalId, Dakota::data_pairs, ApplicationInterface::defaultASV, ApplicationInterface::derived_map(), ApplicationInterface::duplication_detect(), ApplicationInterface::evalCacheFlag, Interface::evalIdCntr, Interface::fineGrainEvalCounters, Interface::fnGradCounter, Interface::fnHessCounter, Interface::fnLabels, Interface::fnValCounter, Response::function_labels(), Interface::init_algebraic_mappings(), ApplicationInterface::init_default_asv(), Interface::init_evaluation_counters(), Interface::interfaceId, ApplicationInterface::manage_failure(), Interface::multiProcEvalFlag, Interface::newEvalIdCntr, Interface::newFnGradCounter, Interface::newFnHessCounter, Interface::newFnValCounter, Interface::outputLevel, ApplicationInterface::parallelLib, ActiveSet::request_vector(), Interface::response_mapping(), ApplicationInterface::restartFileFlag, ApplicationInterface::sharedRespData, and ParallelLibrary::write_restart().

14.7.2.3 const IntResponseMap & synchronize ( ) [protected], [virtual]

executes a blocking schedule for asynchronous evaluations in the beforeSynchCorePRPQueue and returns all jobs

This function provides blocking synchronization for all cases of asynchronous evaluations, including the local asynchronous case (background system call, nonblocking fork, & multithreads), the message passing case, and the hybrid case. Called from derived_synchronize() in derived Model classes.

Reimplemented from Interface.

References Interface::algebraic_mappings(), Interface::algebraicMappings, Interface::asv_mapping(), ApplicationInterface::asynchLocalEvalStatic, ApplicationInterface::asynchronous_local_evaluations(), ApplicationInterface::beforeSynchAlgPRPQueue, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::beforeSynchDuplicateMap, Interface::cachedResponseMap, Interface::coreMappings, ApplicationInterface::evalScheduling, ApplicationInterface::historyDuplicateMap, Interface::ieDedMasterFlag, ApplicationInterface::ieMessagePass, Interface::interfaceId, Interface::interfaceType, ApplicationInterface::master_dynamic_schedule_evaluations(), Interface::multiProcEvalFlag, Interface::outputLevel, ApplicationInterface::peer_dynamic_schedule_evaluations(), ApplicationInterface::peer_static_schedule_evaluations(), Interface::rawResponseMap, Interface::response_mapping(), and ApplicationInterface::sharedRespData.

14.7.2.4 const IntResponseMap & synchronize_nowait ( ) [protected], [virtual]

executes a nonblocking schedule for asynchronous evaluations in the beforeSynchCorePRPQueue and returns a partial set of completed jobs

This function provides nonblocking synchronization for the local asynchronous case and selected nonblocking message passing schedulers. Called from derived_synchronize_nowait() in derived Model classes.

Reimplemented from Interface.

References Interface::algebraic_mappings(), Interface::algebraicMappings, Interface::asv_mapping(), ApplicationInterface::asynchLocalEvalStatic, ApplicationInterface::asynchronous_local_evaluations_nowait(), ApplicationInterface::beforeSynchAlgPRPQueue, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::beforeSynchDuplicateMap, Interface::cachedResponseMap, Interface::coreMappings, ParamResponsePair::eval_id(), ApplicationInterface::evalScheduling, ApplicationInterface::headerFlag, ApplicationInterface::historyDuplicateMap, Interface::ieDedMasterFlag, ApplicationInterface::ieMessagePass, Interface::interfaceId, Interface::interfaceType, Dakota::lookup_by_eval_id(), ApplicationInterface::master_dynamic_schedule_evaluations_nowait(), Interface::multiProcEvalFlag, Interface::outputLevel, ApplicationInterface::peer_dynamic_schedule_evaluations_nowait(), ApplicationInterface::peer_static_schedule_evaluations_nowait(), Interface::rawResponseMap, ParamResponsePair::response(), Interface::response_mapping(), ApplicationInterface::sharedRespData, and Response::update().

14.7.2.5 void serve_evaluations ( ) [protected], [virtual]

run on evaluation servers to serve the iterator master

Invoked by the serve() function in derived Model classes. Passes control to serve_evaluations_synch(), serve_evaluations_asynch(), serve_evaluations_synch_peer(), or serve_evaluations_asynch_peer() according to specified concurrency, partition, and scheduler configuration.

Reimplemented from Interface.

References ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::evalServerId, Interface::ieDedMasterFlag, ApplicationInterface::serve_evaluations_asynch(), ApplicationInterface::serve_evaluations_asynch_peer(), ApplicationInterface::serve_evaluations_synch(), and ApplicationInterface::serve_evaluations_synch_peer().

14.7.2.6 void stop_evaluation_servers ( ) [protected], [virtual]

used by the iterator master to terminate evaluation servers

This code is executed on the iteratorComm rank 0 processor when iteration on a particular model is complete. It sends a termination signal (tag = 0 instead of a valid fn_eval_id) to each of the slave analysis servers. NOTE: This function is called from the Strategy layer even when in serial mode. Therefore, use iteratorCommSize to provide appropriate fall through behavior.

Reimplemented from Interface.

References ParallelLibrary::bcast_e(), ParallelLibrary::free(), ParallelConfiguration::ie_parallel_level(), Interface::ieDedMasterFlag, ParallelLibrary::isend_ie(), ApplicationInterface::iteratorCommSize, Interface::multiProcEvalFlag, ApplicationInterface::numEvalServers, Interface::outputLevel, ParallelLibrary::parallel_configuration(), and ApplicationInterface::parallelLib.

14.7.2.7 void init_communicators_checks (int *max_eval_concurrency*) [protected], [virtual]

perform construct-time error checks on the parallel configuration

Override DirectApplicInterface definition if plug-in to allow batch processing in Plugin{Serial,Parallel}DirectApplicInterface.cpp

Reimplemented in DirectApplicInterface, ProcessHandleApplicInterface, SysCallApplicInterface, and Pybind11Interface.

Referenced by ApplicationInterface::init_communicators().

14.7.2.8 void set_communicators_checks (int *max_eval_concurrency*) [protected], [virtual]

perform run-time error checks on the parallel configuration

Override DirectApplicInterface definition if plug-in to allow batch processing in Plugin{Serial,Parallel}DirectApplicInterface.cpp

Reimplemented in DirectApplicInterface, SerialDirectApplicInterface, SoleilDirectApplicInterface, ParallelDirectApplicInterface, ProcessHandleApplicInterface, SysCallApplicInterface, and Pybind11Interface.

Referenced by ApplicationInterface::set_communicators().

14.7.2.9 void master_dynamic_schedule_analyses ( ) [protected]

blocking dynamic schedule of all analyses within a function evaluation using message passing

This code is called from derived classes to provide the master portion of a master-slave algorithm for the dynamic scheduling of analyses among slave servers. It is patterned after master_dynamic_schedule_evaluations(). It performs no analyses locally and matches either serve_analyses_synch() or serve_analyses_asynch() on the slave servers, depending on the value of asynchLocalAnalysisConcurrency. Dynamic scheduling assigns jobs in 2 passes. The 1st pass gives each server the same number of jobs (equal to asynchLocalAnalysisConcurrency). The 2nd pass assigns the remaining jobs to slave servers as previous jobs are completed. Single- and multilevel parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within ParallelLibrary.

References ApplicationInterface::asynchLocalAnalysisConcurrency, ParallelLibrary::free(), ParallelLibrary::irecv_ea(), ParallelLibrary::isend_ea(), ApplicationInterface::numAnalysisDrivers, ApplicationInterface::numAnalysisServers, ApplicationInterface::parallelLib, ParallelLibrary::waitall(), and ParallelLibrary::waitsome().

Referenced by ProcessHandleApplicInterface::create_evaluation_process(), SysCallApplicInterface::create_evaluation_process(), and DirectApplicInterface::derived_map().

14.7.2.10 void serve_analyses_synch ( ) [protected]

serve the master analysis scheduler and manage one synchronous analysis job at a time

This code is called from derived classes to run synchronous analyses on slave processors. The slaves receive requests (blocking receive), do local derived_map_ac's, and return codes. This is done continuously until a termination signal is received from the master. It is patterned after serve_evaluations_synch().

References ApplicationInterface::analysisCommRank, ParallelLibrary::bcast_a(), ParallelLibrary::isend_ea(), ApplicationInterface::multiProcAnalysisFlag, ApplicationInterface::parallelLib, ParallelLibrary::recv_ea(), ApplicationInterface::synchronous_local_analysis(), and ParallelLibrary::wait().

Referenced by ProcessHandleApplicInterface::create_evaluation_process(), SysCallApplicInterface::create_evaluation_process(), and DirectApplicInterface::derived_map().

14.7.2.11 bool duplication_detect (const Variables & *vars*, Response & *response*, bool *asynch_flag*) [private]

checks data_pairs and beforeSynchCorePRPQueue to see if the current evaluation request has already been performed or queued

Called from map() to check incoming evaluation request for duplication with content of data_pairs and beforeSynchCorePRPQueue. If duplication is detected, return true, else return false. Manage bookkeeping with historyDuplicateMap and beforeSynchDuplicateMap. Note that the list searches can get very expensive if a long list is searched on every new function evaluation (either from a large number of previous jobs, a large number of pending jobs, or both). For this reason, a user request for deactivation of the evaluation cache results in a complete bypass of duplication_detect(), even though a beforeSynchCorePRPQueue search would still be meaningful. Since the intent of this request is to streamline operations, both list searches are bypassed.

References Response::active_set(), ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::beforeSynchDuplicateMap, Response::copy(), Dakota::data_pairs, ParamResponsePair::eval_id(), Interface::evalIdCntr, ApplicationInterface::historyDuplicateMap, Interface::interfaceId, Dakota::lookup_by_val(), ApplicationInterface::nearbyDuplicateDetect, ApplicationInterface::nearbyTolerance, and Response::update().

Referenced by ApplicationInterface::map().

14.7.2.12 void init_default_asv (size_t *num_fns*) [private]

initialize default ASV if needed; this is done at run time due to post-construct time Response size changes.

If the user has specified active_set_vector as off, then map() uses a default ASV which is constant for all function evaluations (so that the user need not check the content of the ASV on each evaluation). Only initialized if needed and not already sized.

References ApplicationInterface::asvControlFlag, ApplicationInterface::defaultASV, ApplicationInterface::gradientType, ApplicationInterface::gradMixedAnalyticIds, ApplicationInterface::hessianType, and ApplicationInterface::hessMixedAnalyticIds.

Referenced by ApplicationInterface::map().

14.7.2.13 void master_dynamic_schedule_evaluations ( ) [private]

blocking dynamic schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a dedicated master partition; executes on iteratorComm master

This code is called from synchronize() to provide the master portion of a master-slave algorithm for the dynamic scheduling of evaluations among slave servers. It performs no evaluations locally and matches either serve_evaluations_synch() or serve_evaluations_asynch() on the slave servers, depending on the value of asynchLocalEvalConcurrency. Dynamic scheduling assigns jobs in 2 passes. The 1st pass gives each server the same number of jobs (equal to asynchLocalEvalConcurrency). The 2nd pass assigns the remaining jobs to slave servers as previous jobs are completed and returned. Single- and multilevel parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within ParallelLibrary. peer

References ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::beforeSynchCorePRPQueue, Dakota::lookup_by_eval_id(), ApplicationInterface::numEvalServers, Interface::outputLevel, ApplicationInterface::parallelLib, ApplicationInterface::receive_evaluation(), ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, ParallelLibrary::waitall(), and ParallelLibrary::waitsome().

Referenced by ApplicationInterface::synchronize().

14.7.2.14 void peer_static_schedule_evaluations ( ) [private]

blocking static schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a peer partition; executes on iteratorComm master

This code runs on the iteratorCommRank 0 processor (the iterator) and is called from synchronize() in order to manage a static schedule for cases where peer 1 must block when evaluating its local job allocation (e.g., single or multiprocessor direct interface evaluations). It matches serve_evaluations_peer() for any other processors within the first evaluation partition and serve_evaluations_{synch,asynch}() for all other evaluation partitions (depending on asynchLocalEvalConcurrency). It performs function evaluations locally for its portion of the job allocation using either asynchronous_local_evaluations() or synchronous_local_evaluations(). Single-level and multilevel parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within ParallelLibrary. The iteratorCommRank 0 processor assigns the static schedule since it is the only processor with access to beforeSynchCorePRPQueue (it runs the iterator and calls synchronize). The alternate design of each peer selecting its own jobs using the modulus operator would be applicable if execution of this function (and therefore the job list) were distributed.

References ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::asynchronous_local_evaluations(), ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::numEvalServers, Interface-

::outputLevel, ApplicationInterface::parallelLib, ApplicationInterface::receive_evaluation(), ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, ApplicationInterface::synchronous_local_evaluations(), and ParallelLibrary::waitall().

Referenced by ApplicationInterface::synchronize().

14.7.2.15 void peer_dynamic_schedule_evaluations ( ) [private]

blocking dynamic schedule of all evaluations in beforeSynchCorePRPQueue using message passing on a peer partition; executes on iteratorComm master

This code runs on the iteratorCommRank 0 processor (the iterator) and is called from synchronize() in order to manage a dynamic schedule, as enabled by nonblocking management of local asynchronous jobs. It matches serve_evaluations_{synch,asynch}() for other evaluation partitions, depending on asynchLocalEvalConcurrency; it does not match serve_evaluations_peer() since, for local asynchronous jobs, the first evaluation partition cannot be multiprocessor. It performs function evaluations locally for its portion of the job allocation using asynchronous_local_evaluations_nowait(). Single-level and multilevel parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within ParallelLibrary.

References ApplicationInterface::assign_asynch_local_queue(), ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::msgPassRunningMap, ApplicationInterface::numEvalServers, Interface::outputLevel, ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, ApplicationInterface::test_local_backfill(), and ApplicationInterface::test_receives_backfill().

Referenced by ApplicationInterface::synchronize().

14.7.2.16 void asynchronous_local_evaluations (PRPQueue & *local_prp_queue*) [private]

perform all jobs in prp_queue using asynchronous approaches on the local processor

This function provides blocking synchronization for the local asynch case (background system call, nonblocking fork, or threads). It can be called from synchronize() for a complete local scheduling of all asynchronous jobs or from peer_{static,dynamic}_schedule_evaluations() to perform a local portion of the total job set. It uses derived_map_asynch() to initiate asynchronous evaluations and wait_local_evaluations() to capture completed jobs, and mirrors the master_dynamic_schedule_evaluations() message passing scheduler as much as possible (wait_local_evaluations() is modeled after MPI_Waitsome()).

References ApplicationInterface::assign_asynch_local_queue(), ApplicationInterface::asynchLocalActivePRPQueue, ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::asynchLocalEvalStatic, ApplicationInterface::batchEval, ApplicationInterface::completionSet, ApplicationInterface::launch_asynch_local(), ApplicationInterface::localServerAssigned, Dakota::lookup_by_eval_id(), ApplicationInterface::numEvalServers, Interface::outputLevel, ApplicationInterface::process_asynch_local(), Interface::rawResponseMap, and ApplicationInterface::wait_local_evaluations().

Referenced by ApplicationInterface::peer_static_schedule_evaluations(), and ApplicationInterface::synchronize().

14.7.2.17 void synchronous_local_evaluations (PRPQueue & *local_prp_queue*) [private]

perform all jobs in prp_queue using synchronous approaches on the local processor

This function provides blocking synchronization for the local synchronous case (foreground system call, blocking fork, or procedure call from derived_map()). It is called from peer_static_schedule_evaluations() to perform a local portion of the total job set.

References ApplicationInterface::broadcast_evaluation(), Interface::currEvalId, ApplicationInterface::derived_map(), ApplicationInterface::manage_failure(), Interface::multiProcEvalFlag, and ApplicationInterface::process_synch_local().

Referenced by ApplicationInterface::peer_static_schedule_evaluations(), and ApplicationInterface::peer_static_schedule_evaluations_nowait().

14.7.2.18 void master_dynamic_schedule_evaluations_nowait ( ) [private]

execute a nonblocking dynamic schedule in a master-slave partition

This code is called from synchronize_nowait() to provide the master portion of a nonblocking master-slave algorithm for the dynamic scheduling of evaluations among slave servers. It performs no evaluations locally and matches either serve_evaluations_synch() or serve_evaluations_asynch() on the slave servers, depending on the value of asynchLocalEvalConcurrency. Dynamic scheduling assigns jobs in 2 passes. The 1st pass gives each server the same number of jobs (equal to asynchLocalEvalConcurrency). The 2nd pass assigns the remaining jobs to slave servers as previous jobs are completed. Single- and multilevel parallel use intra- and inter-communicators, respectively, for send/receive. Specific syntax is encapsulated within ParallelLibrary.

References Dakota::abort_handler(), ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::headerFlag, ApplicationInterface::msgPassRunningMap, ApplicationInterface::numEvalServers, ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, and ApplicationInterface::test_receives_backfill().

Referenced by ApplicationInterface::synchronize_nowait().

14.7.2.19 void peer_static_schedule_evaluations_nowait ( ) [private]

execute a nonblocking static schedule in a peer partition

This code runs on the iteratorCommRank 0 processor (the iterator) and is called from synchronize_nowait() in order to manage a nonblocking static schedule. It matches serve_evaluations_synch() for other evaluation partitions (asynchLocalEvalConcurrency == 1). It performs blocking local function evaluations, one at a time, for its portion of the static schedule and checks for remote completions in between each local completion. Therefore, unlike peer_dynamic_schedule_evaluations_nowait(), this scheduler will always return at least one job. Single-level and multilevel parallel use intra- and inter-communicators, respectively, for send/receive, with specific syntax as encapsulated within ParallelLibrary. The iteratorCommRank 0 processor assigns the static schedule since it is the only processor with access to beforeSynchCorePRPQueue (it runs the iterator and calls synchronize). The alternate design of each peer selecting its own jobs using the modulus operator would be applicable if execution of this function (and therefore the job list) were distributed.

References Dakota::abort_handler(), ApplicationInterface::assign_asynch_local_queue(), ApplicationInterface::assign_asynch_local_queue_nowait(), ApplicationInterface::asynchLocalActivePRPQueue, ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::headerFlag, Interface::interfaceType, Dakota::lookup_by_eval_id(), ApplicationInterface::msgPassRunningMap, Interface::multiProcEvalFlag, ApplicationInterface::nowaitEvalIdRef, ApplicationInterface::numEvalServers, ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, ApplicationInterface::synchronous_local_evaluations(), ApplicationInterface::test_local_backfill(), and ApplicationInterface::test_receives_backfill().

Referenced by ApplicationInterface::synchronize_nowait().

14.7.2.20 void peer_dynamic_schedule_evaluations_nowait ( ) [private]

execute a nonblocking dynamic schedule in a peer partition

This code runs on the iteratorCommRank 0 processor (the iterator) and is called from synchronize_nowait() in order to manage a nonblocking static schedule. It matches serve_evaluations_{synch,asynch}() for other evaluation partitions (depending on asynchLocalEvalConcurrency). It performs nonblocking local function evaluations for its portion of the static schedule using asynchronous_local_evaluations(). Single-level and multilevel parallel use intra- and inter-communicators, respectively, for send/receive, with specific syntax as encapsulated within ParallelLibrary. The iteratorCommRank 0 processor assigns the dynamic schedule since it is the only processor with access to beforeSynchCorePRPQueue (it runs the iterator and calls synchronize). The alternate design of each peer selecting its own jobs using the modulus operator would be applicable if execution of this function (and therefore the job list) were distributed.

References Dakota::abort_handler(), ApplicationInterface::assign_asynch_local_queue(), ApplicationInterface-

::assign_asynch_local_queue_nowait(), ApplicationInterface::asynchLocalActivePRPQueue, ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::beforeSynchCorePRPQueue, ApplicationInterface::headerFlag, Dakota::lookup_by_eval_id(), ApplicationInterface::msgPassRunningMap, ApplicationInterface::numEvalServers, ApplicationInterface::recvBuffers, ApplicationInterface::recvRequests, ApplicationInterface::send_evaluation(), ApplicationInterface::sendBuffers, ApplicationInterface::test_local_backfill(), and ApplicationInterface::test_receives_backfill().

Referenced by ApplicationInterface::synchronize_nowait().

14.7.2.21 void asynchronous_local_evaluations_nowait (PRPQueue & *local_prp_queue*) [private]

launch new jobs in prp_queue asynchronously (if capacity is available), perform nonblocking query of all running jobs, and process any completed jobs (handles both local master- and local peer-scheduling cases)

This function provides nonblocking synchronization for the local asynch case (background system call, nonblocking fork, or threads). It is called from synchronize_nowait() and passed the complete set of all asynchronous jobs (beforeSynchCorePRPQueue). It uses derived_map_asynch() to initiate asynchronous evaluations and test_local_evaluations() to capture completed jobs in nonblocking mode. It mirrors a nonblocking message passing scheduler as much as possible (test_local_evaluations() modeled after MPI_Testsome()). The result of this function is rawResponseMap, which uses eval_id as a key. It is assumed that the incoming local_prp_queue contains only active and new jobs - i.e., all completed jobs are cleared by synchronize_nowait().

Also supports asynchronous local evaluations with static scheduling. This scheduling policy specifically ensures that a completed asynchronous evaluation eval_id is replaced with an equivalent one, modulo asynchLocalEvalConcurrency. In the nowait case, this could render some servers idle if evaluations don't come in eval_id order or some evaluations are cancelled by the caller in between calls. If this function is called with unlimited local eval concurrency, the static scheduling request is ignored.

References ApplicationInterface::assign_asynch_local_queue_nowait(), ApplicationInterface::asynchLocalActivePRPQueue, ApplicationInterface::asynchLocalEvalConcurrency, ApplicationInterface::asynchLocalEvalStatic, ApplicationInterface::headerFlag, and ApplicationInterface::test_local_backfill().

Referenced by ApplicationInterface::synchronize_nowait().

14.7.2.22 void serve_evaluations_synch ( ) [private]

serve the evaluation message passing schedulers and perform one synchronous evaluation at a time

This code is invoked by serve_evaluations() to perform one synchronous job at a time on each slave/peer server. The servers receive requests (blocking receive), do local synchronous maps, and return results. This is done continuously until a termination signal is received from the master (sent via stop_evaluation_servers()).

References ParallelLibrary::bcast_e(), Interface::currEvalId, ApplicationInterface::derived_map(), ApplicationInterface::evalCommRank, ParallelLibrary::isend_ie(), ApplicationInterface::lenResponseMessage, ApplicationInterface::lenVarsActSetMessage, ApplicationInterface::manage_failure(), Interface::multiProcEvalFlag, ApplicationInterface::parallelLib, ParallelLibrary::recv_ie(), MPIPackBuffer::reset(), ApplicationInterface::sharedRespData, and ParallelLibrary::wait().

Referenced by ApplicationInterface::serve_evaluations().

14.7.2.23 void serve_evaluations_synch_peer ( ) [private]

serve the evaluation message passing schedulers and perform one synchronous evaluation at a time as part of the 1st peer

This code is invoked by serve_evaluations() to perform a synchronous evaluation in coordination with the iteratorCommRank 0 processor (the iterator) for static schedules. The bcast() matches either the bcast() in synchronous_local_evaluations(), which is invoked by peer_static_schedule_evaluations(), or the bcast() in map().

References ParallelLibrary::bcast_e(), Interface::currEvalId, ApplicationInterface::derived_map(), ApplicationInterface::lenVarsActSetMessage, ApplicationInterface::manage_failure(), ApplicationInterface::parallelLib, and

ApplicationInterface::sharedRespData.

Referenced by ApplicationInterface::serve_evaluations().

14.7.2.24 void serve_evaluations_asynch ( ) [private]

serve the evaluation message passing schedulers and manage multiple asynchronous evaluations

This code is invoked by serve_evaluations() to perform multiple asynchronous jobs on each slave/peer server. The servers test for any incoming jobs, launch any new jobs, process any completed jobs, and return any results. Each of these components is nonblocking, although the server loop continues until a termination signal is received from the master (sent via stop_evaluation_servers()). In the master-slave case, the master maintains the correct number of jobs on each slave. In the static scheduling case, each server is responsible for limiting concurrency (since the entire static schedule is sent to the peers at start up).

References Dakota::abort_handler(), ApplicationInterface::asynchLocalActivePRPQueue, ApplicationInterface::asynchLocalEvalConcurrency, ParallelLibrary::bcast_e(), ApplicationInterface::completionSet, ApplicationInterface::evalCommRank, ParallelLibrary::irecv_ie(), ApplicationInterface::launch_asynch_local(), ApplicationInterface::lenResponseMessage, ApplicationInterface::lenVarsActSetMessage, Dakota::lookup_by_eval_id(), Interface::multiProcEvalFlag, ApplicationInterface::parallelLib, ParallelLibrary::recv_ie(), ParallelLibrary::send_ie(), ParallelLibrary::test(), and ApplicationInterface::test_local_evaluations().

Referenced by ApplicationInterface::serve_evaluations().

14.7.2.25 void serve_evaluations_asynch_peer ( ) [private]

serve the evaluation message passing schedulers and perform multiple asynchronous evaluations as part of the 1st peer

This code is invoked by serve_evaluations() to perform multiple asynchronous jobs on multiprocessor slave/peer servers. It matches the multiProcEvalFlag bcasts in ApplicationInterface::asynchronous_local_evaluations().

References Dakota::abort_handler(), ApplicationInterface::asynchLocalActivePRPQueue, ApplicationInterface::asynchLocalEvalConcurrency, ParallelLibrary::bcast_e(), ApplicationInterface::completionSet, ApplicationInterface::launch_asynch_local(), ApplicationInterface::lenVarsActSetMessage, Dakota::lookup_by_eval_id(), ApplicationInterface::parallelLib, and ApplicationInterface::test_local_evaluations().

Referenced by ApplicationInterface::serve_evaluations().

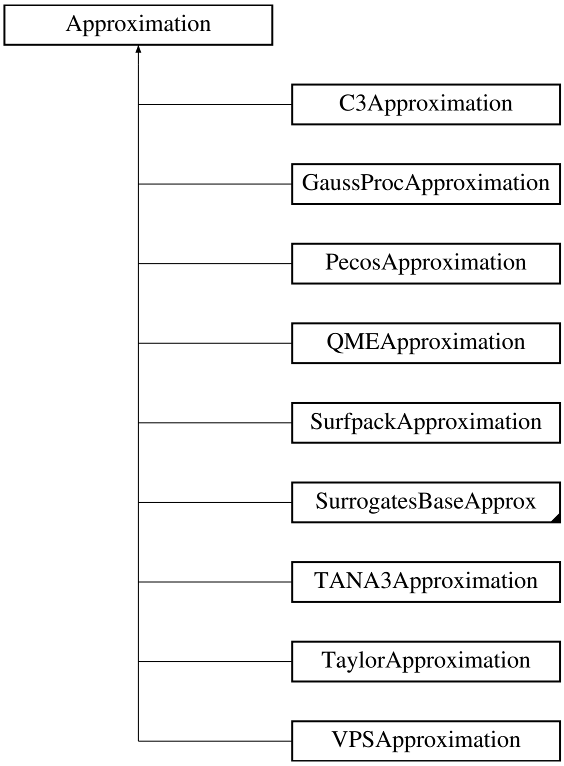
The documentation for this class was generated from the following files:

- ApplicationInterface.hpp
- ApplicationInterface.cpp

14.8 Approximation Class Reference

Base class for the approximation class hierarchy.

Inheritance diagram for Approximation:



Public Member Functions

- Approximation ()

  default constructor
- Approximation (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

  standard constructor for envelope
- Approximation (const SharedApproxData &shared_data)

  alternate constructor
- Approximation (const Approximation &approx)

  copy constructor
- virtual ∼Approximation ()

  destructor
- Approximation operator= (const Approximation &approx)

  assignment operator
- virtual void active_model_key (const Pecos::ActiveKey &sd_key)

  activate an approximation state based on its multi-index key
- virtual void clear_model_keys ()

  reset initial state by removing all model keys for an approximation
- virtual void build ()

  builds the approximation from scratch
- virtual void export_model (const StringArray &var_labels=StringArray(), const String &fn_label="", const String &export_prefix="", const unsigned short export_format=NO_MODEL_FORMAT)

  exports the approximation; if export_format > NO_MODEL_FORMAT, uses all 3 parameters, otherwise extracts these from the Approximation's sharedDataRep to build a filename
- virtual void export_model (const Variables &vars, const String &fn_label="", const String &export_prefix="", const unsigned short export_format=NO_MODEL_FORMAT)

approximation export that generates labels from the passed Variables, since only the derived classes know how the variables are ordered w.r.t. the surrogate build; if export_format > NO_MODEL_FORMAT, uses all 3 parameters, otherwise extracts these from the Approximation's sharedDataRep to build a filename

- virtual void rebuild ()

  rebuilds the approximation incrementally
- virtual void replace (const IntResponsePair &response_pr, size_t fn_index)

  replace the response data
- virtual void pop_coefficients (bool save_data)

  removes entries from end of SurrogateData::{vars,resp}Data (last points appended, or as specified in args)
- virtual void push_coefficients ()

  restores state prior to previous pop()
- virtual void finalize_coefficients ()

  finalize approximation by applying all remaining trial sets
- virtual void clear_current_active_data ()

  clear current build data in preparation for next build
- virtual void combine_coefficients ()

  combine all level approximations into a single aggregate approximation
- virtual void combined_to_active_coefficients (bool clear_combined=true)

  promote combined approximation into active approximation
- virtual void clear_inactive_coefficients ()

  prune inactive coefficients following combination and promotion to active
- virtual Real value (const Variables &vars)

  retrieve the approximate function value for a given parameter vector
- virtual const RealVector & gradient (const Variables &vars)

  retrieve the approximate function gradient for a given parameter vector
- virtual const RealSymMatrix & hessian (const Variables &vars)

  retrieve the approximate function Hessian for a given parameter vector
- virtual Real prediction_variance (const Variables &vars)

  retrieve the variance of the predicted value for a given parameter vector
- virtual Real value (const RealVector &c_vars)

  retrieve the approximate function value for a given parameter vector
- virtual const RealVector & gradient (const RealVector &c_vars)

  retrieve the approximate function gradient for a given parameter vector
- virtual const RealSymMatrix & hessian (const RealVector &c_vars)

  retrieve the approximate function Hessian for a given parameter vector
- virtual Real prediction_variance (const RealVector &c_vars)

  retrieve the variance of the predicted value for a given parameter vector
- virtual Real mean ()

  return the mean of the expansion, where all active vars are random
- virtual Real mean (const RealVector &x)

  return the mean of the expansion for a given parameter vector, where a subset of the active variables are random
- virtual Real combined_mean ()

  return the mean of the combined expansion, where all active vars are random
- virtual Real combined_mean (const RealVector &x)

  return the mean of the combined expansion for a given parameter vector, where a subset of the active variables are random
- virtual const RealVector & mean_gradient ()

  return the gradient of the expansion mean
- virtual const RealVector & mean_gradient (const RealVector &x, const SizetArray &dvv)

  return the gradient of the expansion mean
- virtual Real variance ()

return the variance of the expansion, where all active vars are random
- virtual Real variance (const RealVector &x)

  return the variance of the expansion for a given parameter vector, where a subset of the active variables are random
- virtual const RealVector & **variance_gradient** ()
- virtual const RealVector & **variance_gradient** (const RealVector &x, const SizetArray &dvv)
- virtual Real covariance (Approximation &approx_2)

  return the covariance between two response expansions, treating all variables as random
- virtual Real covariance (const RealVector &x, Approximation &approx_2)

  return the covariance between two response expansions, treating a subset of the variables as random
- virtual Real combined_covariance (Approximation &approx_2)

  return the covariance between two combined response expansions, where all active variables are random
- virtual Real combined_covariance (const RealVector &x, Approximation &approx_2)

  return the covariance between two combined response expansions, where a subset of the active variables are random
- virtual void **compute_moments** (bool full_stats=true, bool combined_stats=false)
- virtual void **compute_moments** (const RealVector &x, bool full_stats=true, bool combined_stats=false)
- virtual const RealVector & **moments** () const
- virtual const RealVector & **expansion_moments** () const
- virtual const RealVector & **numerical_integration_moments** () const
- virtual const RealVector & **combined_moments** () const
- virtual Real **moment** (size_t i) const
- virtual void **moment** (Real mom, size_t i)
- virtual Real **combined_moment** (size_t i) const
- virtual void **combined_moment** (Real mom, size_t i)
- virtual void **clear_component_effects** ()
- virtual void **compute_component_effects** ()
- virtual void **compute_total_effects** ()
- virtual const RealVector & **sobol_indices** () const
- virtual const RealVector & **total_sobol_indices** () const
- virtual ULongULongMap **sparse_sobol_index_map** () const
- virtual bool advancement_available ()

  check if resolution advancement (e.g., order, rank) is available for this approximation instance
- virtual bool diagnostics_available ()

  check if diagnostics are available for this approximation type
- virtual Real diagnostic (const String &metric_type)

  retrieve a single diagnostic metric for the diagnostic type specified
- virtual RealArray cv_diagnostic (const StringArray &metric_types, unsigned num_folds)

  retrieve diagnostic metrics for the diagnostic types specified, applying
- virtual void primary_diagnostics (size_t fn_index)

  compute and print all requested diagnostics and cross-validation
- virtual RealArray challenge_diagnostic (const StringArray &metric_types, const RealMatrix &challenge_-points, const RealVector &challenge_responses)

  compute requested diagnostics for user provided challenge pts
- virtual void challenge_diagnostics (size_t fn_index, const RealMatrix &challenge_points, const RealVector &challenge_responses)

  compute and print all requested diagnostics for user provided challenge pts
- virtual RealVector approximation_coefficients (bool normalized) const

  return the coefficient array computed by build()/rebuild()
- virtual void approximation_coefficients (const RealVector &approx_coeffs, bool normalized)

  set the coefficient array from external sources, rather than computing with build()/rebuild()
- virtual void coefficient_labels (std::vector< std::string > &coeff_labels) const

  print the coefficient array computed in build()/rebuild()
- virtual void print_coefficients (std::ostream &s, bool normalized)

print the coefficient array computed in build()/rebuild()

- virtual int min_coefficients () const

  return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions

- virtual int recommended_coefficients () const

  return the recommended number of samples (unknowns) required to build the derived class approximation type in numVars dimensions

- virtual int num_constraints () const

  return the number of constraints to be enforced via an anchor point

- virtual void **expansion_coefficient_flag** (bool)
- virtual bool **expansion_coefficient_flag** () const
- virtual void **expansion_gradient_flag** (bool)
- virtual bool **expansion_gradient_flag** () const
- virtual void clear_computed_bits ()

  clear tracking of computed moments, due to (expansion) change that invalidates previous results

- virtual void map_variable_labels (const Variables &dfsm_vars)

  if needed, map passed all variable labels to approximation's labels

- int min_points (bool constraint_flag) const

  *return the minimum number of points required to build the approximation type in numVars dimensions. Uses *_-coefficients() and num_constraints().*

- int recommended_points (bool constraint_flag) const

  return the recommended number of samples to build the approximation type in numVars dimensions (default same as min_points)

- void pop_data (bool save_data)

  removes entries from end of SurrogateData::{vars,resp}Data (last points appended, or as specified in args)

- void push_data ()

  restores SurrogateData state prior to previous pop()

- void finalize_data ()

  finalize SurrogateData by applying all remaining trial sets

- const Pecos::SurrogateData & surrogate_data () const

  return approxData

- Pecos::SurrogateData & surrogate_data ()

  return approxData

- void add (const Variables &vars, bool v_copy, const Response &response, size_t fn_index, bool r_copy, bool anchor_flag, int eval_id, size_t key_index=_NPOS)

  create SurrogateData{Vars,Resp} and append to SurrogateData:: {varsData,respData,dataIdentifiers}

- void add (const Real *c_vars, bool v_copy, const Response &response, size_t fn_index, bool r_copy, bool anchor_flag, int eval_id, size_t key_index=_NPOS)

  create SurrogateData{Vars,Resp} and append to SurrogateData:: {varsData,respData,dataIdentifiers}

- void add (const Pecos::SurrogateDataVars &sdv, bool v_copy, const Response &response, size_t fn_index, bool r_copy, bool anchor_flag, int eval_id, size_t key_index=_NPOS)

  create a SurrogateDataResp and append to SurrogateData:: {varsData,respData,dataIdentifiers}

- void add (const Pecos::SurrogateDataVars &sdv, bool v_copy, const Pecos::SurrogateDataResp &sdr, bool r_copy, bool anchor_flag, int eval_id, size_t key_index=_NPOS)

  append to SurrogateData::{varsData,respData,dataIdentifiers}

- void add_array (const RealMatrix &sample_vars, bool v_copy, const RealVector &sample_resp, bool r_copy, size_t key_index=_NPOS)

  add surrogate data from the provided sample and response data, assuming continuous variables and function values only

- void pop_count (size_t count, size_t key_index)

  appends to SurrogateData::popCountStack (number of entries to pop from end of SurrogateData::{vars,resp}Data, based on size of last data append)

- void clear_data ()

clear SurrogateData::{vars,resp}Data for activeKey + embedded keys

- void clear_active_data ()

  clear active approximation data
- void clear_inactive_data ()

  clear inactive approximation data
- void clear_active_popped ()

  clear SurrogateData::popped{Vars,Resp}Trials,popCountStack for activeKey
- void clear_popped ()

  clear SurrogateData::popped{Vars,Resp}Trials,popCountStack for all keys
- void set_bounds (const RealVector &c_l_bnds, const RealVector &c_u_bnds, const IntVector &di_l_bnds, const IntVector &di_u_bnds, const RealVector &dr_l_bnds, const RealVector &dr_u_bnds)

  set approximation lower and upper bounds (currently only used by graphics)
- std::shared_ptr< Approximation > approx_rep () const

  returns approxRep for access to derived class member functions that are not mapped to the top Approximation level

Protected Member Functions

- Approximation (BaseConstructor, const ProblemDescDB &problem_db, const SharedApproxData &shared_-data, const String &approx_label)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- Approximation (NoDBBaseConstructor, const SharedApproxData &shared_data)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- Pecos::SurrogateDataVars variables_to_sdv (const Real ∗sample_c_vars)

  create a SurrogateDataVars instance from a Real∗
- Pecos::SurrogateDataVars variables_to_sdv (const Variables &vars)

  create a SurrogateDataVars instance by extracting data from a Variables object
- Pecos::SurrogateDataResp response_to_sdr (const Response &response, size_t fn_index)

  create a SurrogateDataResp instance by extracting data for a particular QoI from a Response object
- void add (const Pecos::SurrogateDataVars &sdv, bool v_copy, const Pecos::SurrogateDataResp &sdr, bool r_copy, bool anchor_flag)

  tracks a new data point by appending to SurrogateData::{vars,Resp}Data
- void add (int eval_id)

  tracks a new data point by appending to SurrogateData::dataIdentifiers
- void check_points (size_t num_build_pts)

  Check number of build points against minimum required.
- void assign_key_index (size_t key_index)

  extract and assign i-th embedded active key

Protected Attributes

- Pecos::SurrogateData approxData

  contains the variables/response data for constructing a single approximation model (one response function). There is only one SurrogateData instance per Approximation, although it may contain keys for different model forms/resolutions and aggregations (e.g., discrepancies) among forms/resolutions.
- RealVector approxGradient

  gradient of the approximation returned by gradient()
- RealSymMatrix approxHessian

  Hessian of the approximation returned by hessian()
- String approxLabel

  label for approximation, if applicable
- std::shared_ptr< SharedApproxData > sharedDataRep

  contains the approximation data that is shared among the response set

Private Member Functions

- std::shared_ptr< Approximation > get_approx (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

    Used only by the standard envelope constructor to initialize approxRep to the appropriate derived type.
- std::shared_ptr< Approximation > get_approx (const SharedApproxData &shared_data)

    Used only by the alternate envelope constructor to initialize approxRep to the appropriate derived type.

Private Attributes

- std::shared_ptr< Approximation > approxRep

    pointer to the letter (initialized only for the envelope)

14.8.1 Detailed Description

Base class for the approximation class hierarchy.

The Approximation class is the base class for the response data fit approximation class hierarchy in DAKOTA. One instance of an Approximation must be created for each function to be approximated (a vector of Approximations is contained in ApproximationInterface). For memory efficiency and enhanced polymorphism, the approximation hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Approximation) serves as the envelope and one of the derived classes (selected in Approximation::get_approx()) serves as the letter.

14.8.2 Constructor & Destructor Documentation

14.8.2.1 Approximation ( )

default constructor

The default constructor is used in Array<Approximation> instantiations and by the alternate envelope constructor. approxRep is NULL in this case (problem_db is needed to build a meaningful Approximation object).

14.8.2.2 Approximation (ProblemDescDB & *problem_db*, const SharedApproxData & *shared_data*, const String & *approx_label*)

standard constructor for envelope

Envelope constructor only needs to extract enough data to properly execute get_approx, since Approximation(BaseConstructor, problem_db) builds the actual base class data for the derived approximations.

References Dakota::abort_handler(), and Approximation::approxRep.

14.8.2.3 Approximation (const SharedApproxData & *shared_data*)

alternate constructor

This is the alternate envelope constructor for instantiations on the fly. Since it does not have access to problem_db, it utilizes the NoDBBaseConstructor constructor chain.

References Dakota::abort_handler(), and Approximation::approxRep.

14.8.2.4 Approximation (const Approximation & *approx*)

copy constructor

Copy constructor manages sharing of approxRep.

14.8.2.5 Approximation (BaseConstructor , const ProblemDescDB & *problem_db,* const SharedApproxData & *shared_data,* const String & *approx_label*) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_approx() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_approx() again). Since the letter IS the representation, its rep pointer is set to NULL.

14.8.2.6 Approximation (NoDBBaseConstructor , const SharedApproxData & *shared_data*) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_approx() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_approx() again). Since the letter IS the representation, its rep pointer is set to NULL.

14.8.3 Member Function Documentation

14.8.3.1 void build ( ) [virtual]

builds the approximation from scratch

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented in PecosApproximation, C3Approximation, VPSApproximation, GaussProcApproximation, SurfpackApproximation, TaylorApproximation, QMEApproximation, TANA3Approximation, SurrogatesGPApprox, and SurrogatesPolyApprox.

References Approximation::approxData, Approximation::approxRep, and Approximation::check_points().

Referenced by QMEApproximation::build(), TANA3Approximation::build(), TaylorApproximation::build(), Surfpack-Approximation::build(), GaussProcApproximation::build(), VPSApproximation::build(), C3Approximation::build(), PecosApproximation::build(), and Approximation::rebuild().

14.8.3.2 void clear_current_active_data ( ) [inline], [virtual]

clear current build data in preparation for next build

Clear current but preserve hisory for active key (virtual function redefined by {TANA3,QMEA}Approximation to de-mote current while preserving previous points).

Reimplemented in QMEApproximation, and TANA3Approximation.

References Approximation::approxRep, and Approximation::clear_active_data().

Referenced by DiscrepancyCorrection::compute().

14.8.3.3 void add_array (const RealMatrix & *sample_vars,* bool *v_copy,* const RealVector & *sample_resp,* bool *r_copy,* size_t *key_index* = _NPOS)

add surrogate data from the provided sample and response data, assuming continuous variables and function values only

Short cut function (not used by ApproximationInterface).

References Dakota::abort_handler(), Approximation::add(), Approximation::approxRep, Approximation::assign_-key_index(), and Approximation::variables_to_sdv().

14.8.3.4 void clear_data ( ) [inline]

clear SurrogateData::{vars,resp}Data for activeKey + embedded keys

Clears out current + history for each tracked key (not virtual).

References Approximation::approxData, and Approximation::approxRep.

14.8.3.5 std::shared_ptr< Approximation > get_approx (ProblemDescDB & *problem_db,* const SharedApproxData & *shared_data,* const String & *approx_label*) [private]

Used only by the standard envelope constructor to initialize approxRep to the appropriate derived type.

Used only by the envelope constructor to initialize approxRep to the appropriate derived type.

References SharedApproxData::data_rep(), ProblemDescDB::get_bool(), and Dakota::strends().

14.8.3.6 std::shared_ptr< Approximation > get_approx (const SharedApproxData & *shared_data*) [private]

Used only by the alternate envelope constructor to initialize approxRep to the appropriate derived type.

Used only by the envelope constructor to initialize approxRep to the appropriate derived type.

References SharedApproxData::data_rep(), and Dakota::strends().

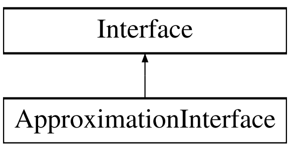
The documentation for this class was generated from the following files:

- DakotaApproximation.hpp
- DakotaApproximation.cpp

14.9 ApproximationInterface Class Reference

Derived class within the interface class hierarchy for supporting approximations to simulation-based results.

Inheritance diagram for ApproximationInterface:



Public Member Functions

- ApproximationInterface (ProblemDescDB &problem_db, const Variables &am_vars, bool am_cache, const String &am_interface_id, const StringArray &fn_labels)

    primary constructor

- ApproximationInterface (const String &approx_type, const UShortArray &approx_order, const Variables &am-_vars, bool am_cache, const String &am_interface_id, size_t num_fns, short data_order, short output_level)

    alternate constructor for instantiations on the fly

- ∼ApproximationInterface ()

    destructor

Protected Member Functions

- void map (const Variables &vars, const ActiveSet &set, Response &response, bool asynch_flag=false)

    the function evaluator: provides an approximate "mapping" from the variables to the responses using functionSurfaces
- int minimum_points (bool constraint_flag) const

    returns the minimum number of samples required to build the functionSurfaces
- int recommended_points (bool constraint_flag) const

    returns the recommended number of samples recommended to build the functionSurfaces
- void active_model_key (const Pecos::ActiveKey &key)

    activate an approximation state based on its key
- void clear_model_keys ()

    reset initial state by removing all model keys for an approximation
- void approximation_function_indices (const SizetSet &approx_fn_indices)

    set the (currently active) approximation function index set
- void update_approximation (const Variables &vars, const IntResponsePair &response_pr)
- void update_approximation (const RealMatrix &samples, const IntResponseMap &resp_map)
- void update_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map)
- void append_approximation (const Variables &vars, const IntResponsePair &response_pr)
- void append_approximation (const RealMatrix &samples, const IntResponseMap &resp_map)
- void append_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map)
- void append_approximation (const IntVariablesMap &vars_map, const IntResponseMap &resp_map)
- void replace_approximation (const IntResponsePair &response_pr)

    replace the response for a single point within an existing approximation
- void replace_approximation (const IntResponseMap &resp_map)

    replace responses for multiple points within an existing approximation
- void track_evaluation_ids (bool track)

    assigns trackEvalIds to activate tracking of evaluation ids within surrogate data, enabling id-based lookups for data replacement
- void build_approximation (const RealVector &c_l_bnds, const RealVector &c_u_bnds, const IntVector &di_l_-bnds, const IntVector &di_u_bnds, const RealVector &dr_l_bnds, const RealVector &dr_u_bnds)
- void export_approximation ()
- void rebuild_approximation (const BitArray &rebuild_fns)
- void pop_approximation (bool save_data)
- void push_approximation ()
- bool push_available ()

    queries the approximation for the ability to retrieve a previous increment
- void finalize_approximation ()

    finalizes the approximation by applying all trial increments
- void combine_approximation ()

    combine the current approximation with previously stored data sets
- void combined_to_active (bool clear_combined=true)

    promote the combined approximation to the currently active one
- void clear_inactive ()

    clear inactive approximation data
- void clear_current_active_data ()

    clears current data from an approximation interface
- void clear_active_data ()

    clears all data from an approximation interface
- SharedApproxData & shared_approximation ()

    retrieve the SharedApproxData within an ApproximationInterface
- std::vector< Approximation > & approximations ()

    retrieve the Approximations within an ApproximationInterface

- const Pecos::SurrogateData & approximation_data (size_t fn_index)

  retrieve the approximation data from a particular Approximation within an ApproximationInterface
- const RealVectorArray & approximation_coefficients (bool normalized=false)

  retrieve the approximation coefficients from each Approximation within an ApproximationInterface
- void approximation_coefficients (const RealVectorArray &approx_coeffs, bool normalized=false)

  set the approximation coefficients within each Approximation within an ApproximationInterface
- const RealVector & approximation_variances (const Variables &vars)

  retrieve the approximation variances from each Approximation within an ApproximationInterface
- bool formulation_updated () const

  query for change in approximation formulation
- void formulation_updated (bool update)

  assign an updated status for approximation formulation to force rebuild
- bool advancement_available ()

  query for available advancements in approximation resolution controls
- Real2DArray cv_diagnostics (const StringArray &metrics, unsigned num_folds)

  approximation cross-validation quality metrics per response function
- Real2DArray **challenge_diagnostics** (const StringArray &metric_types, const RealMatrix &challenge_pts, const RealVector &challenge_resps)
- const IntResponseMap & synchronize ()

  recovers data from a series of asynchronous evaluations (blocking)
- const IntResponseMap & synchronize_nowait ()

  recovers data from a series of asynchronous evaluations (nonblocking)

Private Member Functions

- void mixed_add (const Variables &vars, const IntResponsePair &response_pr, bool anchor)

  add variables/response data to functionSurfaces using a mixture of shallow and deep copies
- void mixed_add (const Real *c_vars, const IntResponsePair &response_pr, bool anchor)

  add variables/response data to functionSurfaces using a mixture of shallow and deep copies
- void shallow_add (const Variables &vars, const IntResponsePair &response_pr, bool anchor)

  add variables/response data to functionSurfaces using a shallow copy
- void sample_to_variables (const Real *sample_c_vars, size_t num_cv, Variables &vars)

  populate continuous variables within vars from sample_c_vars
- void update_pop_counts (const IntResponsePair &response_pr)

  append to the stack of pop counts within each of the functionSurfaces based on the active set definition within a single incoming response
- void update_pop_counts (const IntResponseMap &resp_map)

  append to the stack of pop counts within each of the functionSurfaces based on the active set definitions within a map of incoming responses
- PRPCacheCIter cache_lookup (const Variables &vars, int eval_id, const Response &response)

  helper to find a cached PRP record in data_pairs
- PRPCacheCIter cache_lookup (const Real *vars, size_t num_v, int eval_id, const Response &response)

  helper to find a cached PRP record in data_pairs
- void check_id (int id1, int id2)

  verify consistency between two evaluation identifiers
- void restore_data_key ()

  following Approximation::add() and Approximation::pop_count() operations, which may enumerate multiple embedded keys, restore the active approxData to the nominal key
- void read_challenge_points ()

  Load approximation test points from user challenge points file.

Private Attributes

- SizetSet approxFnIndices
  for incomplete approximation sets, this array specifies the response function subset that is approximated
- SharedApproxData sharedData
  data that is shared among all functionSurfaces
- std::vector< Approximation > functionSurfaces
  list of approximations, one per response function
- RealVectorArray functionSurfaceCoeffs
  array of approximation coefficient vectors, one per response function
- RealVector functionSurfaceVariances
  vector of approximation variances, one value per response function
- bool trackEvalIds
  flag to activate the tracking of evaluation ids within surrogate data
- String challengeFile
  data file for user-supplied challenge data (per interface, since may contain multiple responses)
- unsigned short challengeFormat
  tabular format of the challenge points file
- bool challengeUseVarLabels
  whether to validate variable labels in header
- bool challengeActiveOnly
  whether to import active only
- RealMatrix challengePoints
  container for the challenge points data (variables only)
- RealMatrix challengeResponses
  container for the challenge points data (responses only)
- Variables actualModelVars
  copy of the actualModel variables object used to simplify conversion among differing variable views
- bool actualModelCache
  indicates usage of an evaluation cache by the actualModel
- String actualModelInterfaceId
  the interface id from the actualModel used for ordered PRPCache lookups
- IntResponseMap beforeSynchResponseMap
  bookkeeping map to catalogue responses generated in map() for use in synchronize() and synchronize_nowait(). This supports pseudo-asynchronous operations (approximate responses are always computed synchronously, but asynchronous virtual functions are supported through bookkeeping).

Static Private Attributes

- static size_t approxIdNum = 0
  counter for giving unique names to approximation interfaces

Additional Inherited Members

14.9.1 Detailed Description

Derived class within the interface class hierarchy for supporting approximations to simulation-based results.

ApproximationInterface provides an interface class for building a set of global/local/multipoint approximations and performing approximate function evaluations using them. It contains a list of Approximation objects, one for each response function.

14.9.2 Member Function Documentation

14.9.2.1 void update_approximation (const Variables & *vars,* const IntResponsePair & *response_pr*) [protected], [virtual]

This function populates/replaces each Approximation::anchorPoint with the incoming variables/response data point.

Reimplemented from Interface.

References ApproximationInterface::actualModelCache, ApproximationInterface::cache_lookup(), Dakota::data_pairs, ApproximationInterface::mixed_add(), ApproximationInterface::restore_data_key(), and ApproximationInterface::shallow_add().

14.9.2.2 void update_approximation (const RealMatrix & *samples,* const IntResponseMap & *resp_map*) [protected], [virtual]

This function populates/replaces each Approximation::currentPoints with the incoming variables/response arrays.

Reimplemented from Interface.

References Dakota::abort_handler(), ApproximationInterface::actualModelCache, ApproximationInterface::approxFnIndices, ApproximationInterface::cache_lookup(), ApproximationInterface::clear_active_data(), Dakota::data_pairs, ApproximationInterface::functionSurfaces, ApproximationInterface::mixed_add(), ApproximationInterface::restore_data_key(), and ApproximationInterface::shallow_add().

14.9.2.3 void update_approximation (const VariablesArray & *vars_array,* const IntResponseMap & *resp_map*) [protected], [virtual]

This function populates/replaces each Approximation::currentPoints with the incoming variables/response arrays.

Reimplemented from Interface.

References Dakota::abort_handler(), ApproximationInterface::actualModelCache, ApproximationInterface::approxFnIndices, ApproximationInterface::cache_lookup(), ApproximationInterface::clear_active_data(), Dakota::data_pairs, ApproximationInterface::functionSurfaces, ApproximationInterface::mixed_add(), ApproximationInterface::restore_data_key(), and ApproximationInterface::shallow_add().

14.9.2.4 void append_approximation (const Variables & *vars,* const IntResponsePair & *response_pr*) [protected], [virtual]

This function appends to each Approximation::currentPoints with one incoming variables/response data point.

Reimplemented from Interface.

References ApproximationInterface::actualModelCache, ApproximationInterface::cache_lookup(), Dakota::data_pairs, ApproximationInterface::mixed_add(), ApproximationInterface::restore_data_key(), ApproximationInterface::shallow_add(), and ApproximationInterface::update_pop_counts().

14.9.2.5 void append_approximation (const RealMatrix & *samples,* const IntResponseMap & *resp_map*) [protected], [virtual]

This function appends to each Approximation::currentPoints with multiple incoming variables/response data points.

Reimplemented from Interface.

References Dakota::abort_handler(), ApproximationInterface::actualModelCache, ApproximationInterface::cache_lookup(), Dakota::data_pairs, ApproximationInterface::mixed_add(), ApproximationInterface::restore_data_key(), ApproximationInterface::shallow_add(), and ApproximationInterface::update_pop_counts().

14.9.2.6 void append_approximation (const VariablesArray & *vars_array,* const IntResponseMap & *resp_map*) [protected], [virtual]

This function appends to each Approximation::currentPoints with multiple incoming variables/response data points.

Reimplemented from Interface.

References Dakota::abort_handler(), ApproximationInterface::actualModelCache, ApproximationInterface::cache_lookup(), Dakota::data_pairs, ApproximationInterface::mixed_add(), ApproximationInterface::restore_data_key(), ApproximationInterface::shallow_add(), and ApproximationInterface::update_pop_counts().

14.9.2.7 void append_approximation (const IntVariablesMap & *vars_map,* const IntResponseMap & *resp_map*) [protected], [virtual]

This function appends to each Approximation::currentPoints with multiple incoming variables/response data points.

Reimplemented from Interface.

References Dakota::abort_handler(), ApproximationInterface::actualModelCache, ApproximationInterface::cache_lookup(), ApproximationInterface::check_id(), Dakota::data_pairs, ApproximationInterface::mixed_add(), ApproximationInterface::restore_data_key(), ApproximationInterface::shallow_add(), and ApproximationInterface::update_pop_counts().

14.9.2.8 void build_approximation (const RealVector & *c_l_bnds,* const RealVector & *c_u_bnds,* const IntVector & *di_l_bnds,* const IntVector & *di_u_bnds,* const RealVector & *dr_l_bnds,* const RealVector & *dr_u_bnds*) [protected], [virtual]

This function finds the coefficients for each Approximation based on the data passed through update_approximation() calls. The bounds are used only for graphics visualization.

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, SharedApproxData::build(), ApproximationInterface::challengeFile, ApproximationInterface::challengePoints, ApproximationInterface::challengeResponses, ApproximationInterface::functionSurfaces, ApproximationInterface::read_challenge_points(), SharedApproxData::set_bounds(), and ApproximationInterface::sharedData.

14.9.2.9 void export_approximation ( ) [protected], [virtual]

This function calls export on each approximation

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, and ApproximationInterface::functionSurfaces.

14.9.2.10 void rebuild_approximation (const BitArray & *rebuild_fns*) [protected], [virtual]

This function updates the coefficients for each Approximation based on data increments provided by {update,append}_approximation().

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, ApproximationInterface::functionSurfaces, SharedApproxData::rebuild(), and ApproximationInterface::sharedData.

14.9.2.11 void pop_approximation (bool *save_data*) [inline], [protected], [virtual]

This function removes data provided by a previous append_approximation() call, possibly different numbers for each function, or as specified in pop_count, which is assumed to be the same for all functions.

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, ApproximationInterface::functionSurfaces, SharedApproxData::pop(), Approximation::pop_coefficients(), Approximation::pop_data(), and ApproximationInterface::sharedData.

14.9.2.12 void push_approximation ( ) [inline], [protected], [virtual]

This function updates the coefficients for each Approximation based on data increments provided by {update,append}_approximation().

Reimplemented from Interface.

References ApproximationInterface::approxFnIndices, ApproximationInterface::functionSurfaces, SharedApproxData::post_push(), SharedApproxData::pre_push(), Approximation::push_coefficients(), Approximation::push_data(), and ApproximationInterface::sharedData.

14.9.2.13 void restore_data_key ( ) [inline], [private]

following Approximation::add() and Approximation::pop_count() operations, which may enumerate multiple embedded keys, restore the active approxData to the nominal key

Restore active key in approxData using shared key.

References Approximation::active_model_key(), SharedApproxData::active_model_key(), ApproximationInterface::approxFnIndices, ApproximationInterface::functionSurfaces, ApproximationInterface::sharedData, and Approximation::surrogate_data().

Referenced by ApproximationInterface::append_approximation(), and ApproximationInterface::update_approximation().

14.9.2.14 void read_challenge_points ( ) [private]

Load approximation test points from user challenge points file.

Challenge data defaults to active/inactive, but user can override to active only.

References ApproximationInterface::actualModelVars, ApproximationInterface::challengeActiveOnly, ApproximationInterface::challengeFile, ApproximationInterface::challengeFormat, ApproximationInterface::challengePoints, ApproximationInterface::challengeResponses, ApproximationInterface::challengeUseVarLabels, Variables::copy(), ApproximationInterface::functionSurfaces, Interface::interface_id(), and Interface::outputLevel.

Referenced by ApproximationInterface::build_approximation().

14.9.3 Member Data Documentation

14.9.3.1 std::vector<Approximation> functionSurfaces [private]

list of approximations, one per response function

This formulation allows the use of mixed approximations (i.e., different approximations used for different response functions), although the input specification is not currently general enough to support it.

Referenced by ApproximationInterface::active_model_key(), ApproximationInterface::advancement_available(), ApproximationInterface::approximation_coefficients(), ApproximationInterface::approximation_data(), ApproximationInterface::approximation_variances(), ApproximationInterface::ApproximationInterface(), ApproximationInterface::approximations(), ApproximationInterface::build_approximation(), ApproximationInterface::clear_active_data(), ApproximationInterface::clear_current_active_data(), ApproximationInterface::clear_inactive(), ApproximationInterface::clear_model_keys(), ApproximationInterface::combine_approximation(), ApproximationInterface::combined_to_active(), ApproximationInterface::cv_diagnostics(), ApproximationInterface::export_approximation(), ApproximationInterface::finalize_approximation(), ApproximationInterface::map(), ApproximationInterface::minimum_points(), ApproximationInterface::mixed_add(), ApproximationInterface::pop_approximation(), Approximation-

Interface::push_approximation(), ApproximationInterface::read_challenge_points(), ApproximationInterface::rebuild_approximation(), ApproximationInterface::recommended_points(), ApproximationInterface::replace_approximation(), ApproximationInterface::restore_data_key(), ApproximationInterface::shallow_add(), ApproximationInterface::update_approximation(), and ApproximationInterface::update_pop_counts().

The documentation for this class was generated from the following files:

- ApproximationInterface.hpp
- ApproximationInterface.cpp

14.10 APPSEvalMgr Class Reference

Evaluation manager class for APPSPACK.

Inherits Executor.

Public Member Functions

- APPSEvalMgr (Optimizer &, Model &model)
  constructor
- ∼APPSEvalMgr ()
  destructor
- bool isReadyForWork () const
  tells APPS whether or not there is a processor available to perform a function evaluation
- bool submit (const int apps_tag, const HOPSPACK::Vector &apps_xtrial, const HOPSPACK::EvalRequestType apps_request)
  performs a function evaluation at APPS-provided x_in
- int recv (int &apps_tag, HOPSPACK::Vector &apps_f, HOPSPACK::Vector &apps_cEqs, HOPSPACK::Vector &apps_cIneqs, string &apps_msg)
  returns a function value to APPS
- std::string getEvaluatorType (void) const
  return the type of the Dakota linked evaluator
- void printDebugInfo (void) const
  empty implementation of debug info needed to complete the interface
- void printTimingInfo (void) const
  empty implementation of timing info needed to complete the interface
- void set_asynch_flag (const bool dakotaAsynchFlag)
  publishes whether or not to do asynchronous evaluations
- void set_blocking_synch (const bool blockingSynchFlag)
  publishes whether or not APPS is operating synchronously
- void set_total_workers (const int numDakotaWorkers)
  publishes the number of processors available for function evaluations

Private Attributes

- Optimizer & dakOpt
  reference to the DakotaOptimizer
- Model & iteratedModel
  reference to the APPSOptimizer's model passed in the constructor
- bool modelAsynchFlag
  flag for asynchronous function evaluations
- bool blockingSynch

flag for APPS synchronous behavior

- int numWorkersUsed

  number of processors actively performing function evaluations
- int numWorkersTotal

  total number of processors available for performing function evaluations
- RealVector xTrial

  trial iterate
- std::map< int, int > tagList

  map of DAKOTA eval id to APPS eval id (for asynchronous evaluations)
- std::map< int, RealVector > functionList

  map of APPS eval id to responses (for synchronous evaluations)
- IntResponseMap dakotaResponseMap

  map of DAKOTA responses returned by synchronize_nowait()

14.10.1 Detailed Description

Evaluation manager class for APPSPACK.

The APPSEvalMgr class is derived from APPSPACK's Executor class. It implements the methods of that class in such away that allows DAKOTA to manage the computation of responses instead of APPS. Iterate and response values are passed between Dakota and APPSPACK via this interface.

14.10.2 Constructor & Destructor Documentation

14.10.2.1 APPSEvalMgr (Optimizer & *opt,* Model & *model*)

constructor

Evaluation manager class for APPSPACK.

The APPSEvalMgr class is derived from APPSPACK's Executor class. It implements the methods of that class in such away that allows DAKOTA to manage the computation of responses instead of APPS. Iterate and response values are passed between Dakota and APPSPACK via this interface.

14.10.3 Member Function Documentation

14.10.3.1 bool isReadyForWork ( ) const

tells APPS whether or not there is a processor available to perform a function evaluation

Check to see if all processors available for function evaluations are being used. If not, tell APPS that one is available.

References APPSEvalMgr::numWorkersTotal, and APPSEvalMgr::numWorkersUsed.

14.10.3.2 bool submit (const int *apps_tag,* const HOPSPACK::Vector & *apps_xtrial,* const HOPSPACK::EvalRequestType *apps_request*)

performs a function evaluation at APPS-provided x_in

Convert APPSPACK vector of variables to DAKOTA vector of variables and perform function evaluation asynchronously or not as specified in the DAKOTA input deck. If evaluation is asynchronous, map the dakota id to the APPS tag. If evaluation is synchronous, map the responses to the APPS tag.

References Model::current_response(), Model::current_variables(), Model::evaluate(), Model::evaluate_nowait(), Model::evaluation_id(), Response::function_values(), APPSEvalMgr::functionList, APPSEvalMgr::iteratedModel, APPSEvalMgr::modelAsynchFlag, APPSEvalMgr::numWorkersTotal, APPSEvalMgr::numWorkersUsed, and APPSEvalMgr::tagList.

14.10.3.3 int recv (int & *apps_tag,* HOPSPACK::Vector & *apps_f,* HOPSPACK::Vector & *apps_cEqs,* HOPSPACK::Vector & *apps_cIneqs,* string & *apps_msg*)

returns a function value to APPS

Retrieve a set of reponse values, convert to APPS data structures, and return them to APPS. APPS tags are tied to corresponding responses using the appropriate (i.e., asynchronous or synchronous) map.

References APPSEvalMgr::blockingSynch, APPSEvalMgr::dakOpt, APPSEvalMgr::dakotaResponseMap, APPSEvalMgr::functionList, Optimizer::get_responses_from_dakota(), APPSEvalMgr::iteratedModel, APPSEvalMgr::modelAsynchFlag, APPSEvalMgr::numWorkersUsed, Model::synchronize(), Model::synchronize_nowait(), and APPSEvalMgr::tagList.

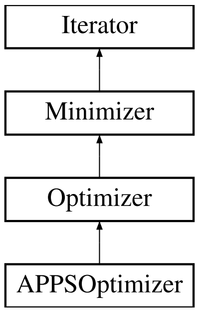
The documentation for this class was generated from the following files:

- APPSEvalMgr.hpp
- APPSEvalMgr.cpp

14.11 APPSOptimizer Class Reference

Wrapper class for HOPSPACK.

Inheritance diagram for APPSOptimizer:



Public Member Functions

- APPSOptimizer (ProblemDescDB &problem_db, Model &model)

  constructor
- APPSOptimizer (Model &model)

  alternate constructor for on-the-fly instantiation without ProblemDescDB
- APPSOptimizer ()

  alternate constructor for even more rudimentary on-the-fly instantiation
- ∼APPSOptimizer ()

  destructor
- void initialize_run ()
- void core_run ()

  compute the optimal solution

Protected Member Functions

- void set_apps_parameters ()

  sets options for specific methods based on user specifications
- void set_apps_traits ()

sets traits for specific TPL

- void initialize_variables_and_constraints ()

    initializes problem variables and constraints

Protected Attributes

- int numTotalVars

    Total across all types of variables.
- HOPSPACK::ParameterList params

    Pointer to APPS parameter list.
- HOPSPACK::ParameterList * problemParams

    Pointer to APPS problem parameter sublist.
- HOPSPACK::ParameterList * linearParams

    Pointer to APPS linear constraint parameter sublist.
- HOPSPACK::ParameterList * mediatorParams

    Pointer to APPS mediator parameter sublist.
- HOPSPACK::ParameterList * citizenParams

    Pointer to APPS citizen/algorithm parameter sublist.
- APPSEvalMgr * evalMgr

    Pointer to the APPS evaluation manager object.

Additional Inherited Members

14.11.1 Detailed Description

Wrapper class for HOPSPACK.

The APPSOptimizer class provides a wrapper for HOPSPACK, a Sandia-developed C++ library for generalized pattern search. HOPSPACK defaults to a coordinate pattern search but also allows for augmented search patterns. It can solve problems with bounds, linear constraints, and general nonlinear constraints. APPSOptimizer uses an APPSEvalMgr object to manage the function evaluations.

The user input mappings are as follows: `output` `max_function_evaluations`, `constraint_tol` `initial_delta`, `contraction_factor`, `variable_tolerance`, `solution_target`, `synchronization`, `merit_function`, `constraint_penalty`, and `smoothing_factor` are mapped into HOPS's "`Display`", "Maximum Evaluations", "Active Tolerance"/"Nonlinear Active Tolerance", "Initial Step", "Contraction Factor", "Step Tolerance", "Objective Target", "Synchronous Evaluations", "Penalty Function", "Penalty Parameter", and "Penalty Smoothing Value" data attributes. Refer to the HOPS web site (https://software.sandia.gov/trac/hopspack) for additional information on HOPS objects and controls.

14.11.2 Member Function Documentation

14.11.2.1 void initialize_run ( ) [virtual]

Allows us to initialize nonlinear equality constraint maps before inequality ones, ie a workaround in need of traits to specify constraint maps packing order - RWH

Reimplemented from Iterator.

References Optimizer::initialize_run(), and Minimizer::numNonlinearIneqConstraints.

14.11.2.2 void core_run ( ) [virtual]

compute the optimal solution

core_run redefines the Optimizer virtual function to perform the optimization using HOPS. It first sets up the problem data, then executes minimize() on the HOPS optimizer, and finally catalogues the results.

Reimplemented from Iterator.

References Model::asynch_flag(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Optimizer::constraintMapIndices, Optimizer::constraintMapMultipliers, Optimizer::constraintMapOffsets, APPSOptimizer::evalMgr, Model::evaluation_capacity(), APPSOptimizer::initialize_variables_and_constraints(), Iterator::iteratedModel, Optimizer::localObjectiveRecast, APPSOptimizer::numTotalVars, Minimizer::numUserPrimaryFns, APPSOptimizer::params, APPSEvalMgr::set_asynch_flag(), and APPSEvalMgr::set_total_workers().

14.11.2.3 void set_apps_parameters ( ) [protected]

sets options for specific methods based on user specifications

Set all of the HOPS algorithmic parameters as specified in the DAKOTA input deck. This is called at construction time.

References APPSOptimizer::citizenParams, Minimizer::constraintTol, APPSOptimizer::evalMgr, ProblemDescDB::get_real(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), ProblemDescDB::is_null(), APPSOptimizer::linearParams, Iterator::maxEvalConcurrency, Iterator::maxFunctionEvals, APPSOptimizer::mediatorParams, Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, Iterator::outputLevel, APPSOptimizer::params, Iterator::probDescDB, APPSOptimizer::problemParams, APPSEvalMgr::set_blocking_synch(), and Dakota::SZ_MAX.

Referenced by APPSOptimizer::APPSOptimizer().

14.11.2.4 void initialize_variables_and_constraints ( ) [protected]

initializes problem variables and constraints

Set the variables and constraints as specified in the DAKOTA input deck. This is done at run time.

References Optimizer::constraintMapIndices, Iterator::iteratedModel, APPSOptimizer::linearParams, Minimizer::numContinuousVars, Minimizer::numDiscreteIntVars, Minimizer::numDiscreteRealVars, Minimizer::numDiscreteStringVars, Minimizer::numLinearEqConstraints, Minimizer::numLinearIneqConstraints, Minimizer::numNonlinearEqConstraints, APPSOptimizer::numTotalVars, and APPSOptimizer::problemParams.

Referenced by APPSOptimizer::core_run().

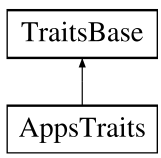
The documentation for this class was generated from the following files:

- APPSOptimizer.hpp
- APPSOptimizer.cpp

14.12 AppsTraits Class Reference

HOPSPACK-specific traits class.

Inheritance diagram for AppsTraits:



Public Types

- typedef HOPSPACK::Hopspack **OptT**
- typedef HOPSPACK::Vector **VecT**
- typedef HOPSPACK::Matrix **MatT**

Public Member Functions

- AppsTraits ()
  default constructor
- virtual ∼AppsTraits ()
  destructor
- virtual bool is_derived ()
  A temporary query used in the refactor.
- bool supports_continuous_variables ()
  Return the flag indicating whether method supports continuous variables.
- bool supports_discrete_variables ()
  Return the flag indicating whether method supports discrete variables.
- bool supports_linear_equality ()
  Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()
  Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()
  Return the flag indicating whether method supports nonlinear equalities.
- NONLINEAR_EQUALITY_FORMAT nonlinear_equality_format ()
  Return the format used for nonlinear equality constraints.
- bool supports_nonlinear_inequality ()
  Return the flag indicating whether method supports nonlinear inequalities.
- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()
  Return the format used for nonlinear inequality constraints.

Static Public Member Functions

- static double **noValue** ()
- static double **getBestObj** (const OptT &)
- static void **copy_matrix_data** (const RealMatrix &source, HOPSPACK::Matrix &target)

14.12.1 Detailed Description

HOPSPACK-specific traits class.

```
AppsTraits specializes some traits accessors by over-riding the default
```

accessors in TraitsBase.

The documentation for this class was generated from the following files:

- APPSOptimizer.hpp
- APPSOptimizer.cpp

14.13 ApreproWriter Class Reference

Utility used in derived write_core to write in aprepro format.

Public Member Functions

- template<typename ArrayType >
  void **operator()** (std::ostream &s, size_t start_index, size_t num_items, const ArrayType &array_data, String-MultiArrayConstView label_array)

14.13.1 Detailed Description

Utility used in derived write_core to write in aprepro format.

The documentation for this class was generated from the following file:

- DakotaVariables.hpp

14.14 AttachScaleVisitor Class Reference

Objects of this class are called by boost::appy_visitor to add dimension scales (RealScale or StringScale) to HDF5 datasets.

Inherits static_visitor<>.

Public Member Functions

- AttachScaleVisitor (const StrStrSizet &iterator_id, const StringArray &location, const int &dim, const String &dset_name, const std::shared_ptr< HDF5IOHelper > &hdf5_stream)

  Construct with context for attaching the scale, including the iterator and location used to construct the scale, the dimension and name of the dataset to attach the scale to, the HDF5IOHelper instance.
- void operator() (const RealScale &scale)

  Called by boost::apply_vistitor to process a RealScale.
- void operator() (const StringScale &scale)

  Called by boost::apply_vistitor to process a StringScale.
- void operator() (const IntegerScale &scale)

  Called by boost::apply_vistitor to process an IntegerScale.

Private Attributes

- StrStrSizet iteratorID

  Iterator ID for the method and execuation.
- StringArray location

  Location used to create the dataset.
- int dimension

  Dimension of the dataset to attach the scale to.
- String dsetName

  Name of the dataset to attach the scale to.
- std::shared_ptr< HDF5IOHelper > hdf5Stream

  Instance of HDF5IOHelper.

14.14.1 Detailed Description

Objects of this class are called by boost::appy_visitor to add dimension scales (RealScale or StringScale) to HDF5 datasets.

The documentation for this class was generated from the following file:

- ResultsDBHDF5.hpp

14.15 BaseConstructor Struct Reference

Dummy struct for overloading letter-envelope constructors.

Public Member Functions

- BaseConstructor (int=0)

  C++ structs can have constructors.

14.15.1 Detailed Description

Dummy struct for overloading letter-envelope constructors.

BaseConstructor is used to overload the constructor for the base class portion of letter objects. It avoids infinite recursion (Coplien p.139) in the letter-envelope idiom by preventing the letter from instantiating another envelope. Putting this struct here avoids circular dependencies.

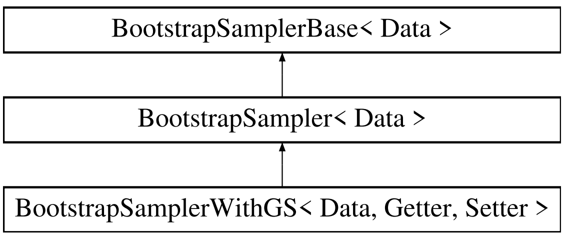
The documentation for this struct was generated from the following file:

- dakota_global_defs.hpp

14.16 BootstrapSampler< Data > Class Template Reference

Actual boostrap sampler implementation for common data types.

Inheritance diagram for BootstrapSampler< Data >:



Public Member Functions

- BootstrapSampler (const Data &orig_data, size_t block_size=1)

  Constructor for the sampler.
- virtual ~BootstrapSampler ()

  Destructor.
- virtual void operator() (size_t num_samp, Data &bootstrapped_sample)

  Generate and store a new boostrapped sample into bootstrapped_sample.

Protected Attributes

- size_t blockSize

  Size of the block defining a sample.

Additional Inherited Members

14.16.1 Detailed Description

template<typename Data>class Dakota::BootstrapSampler< Data >

Actual boostrap sampler implementation for common data types.

Template requires the given type to support an STL-like interface, including a size method and begin and end methods returning random access iterators

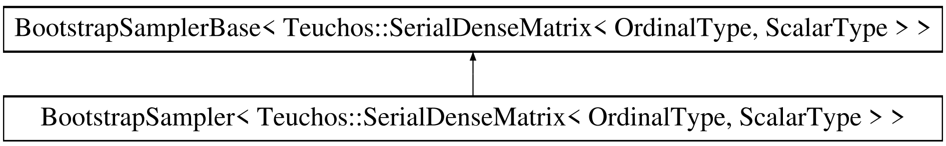
The documentation for this class was generated from the following file:

- BootstrapSampler.hpp

14.17 BootstrapSampler< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > > Class Template Reference

Bootstrap sampler that is specialized to allow for the boostrapping of RealMatrix.

Inheritance diagram for BootstrapSampler< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > >:



Public Types

- typedef
  Teuchos::SerialDenseMatrix
  < OrdinalType, ScalarType > MatType

  Convenience definition.

Public Member Functions

- BootstrapSampler (const MatType &orig_data, size_t block_size=1)

  Constructor for the sampler.
- virtual ~BootstrapSampler ()

  Destructor.
- virtual void operator() (size_t num_samp, MatType &bootstrapped_sample)

  Generate and store a new boostrapped sample into bootstrapped_sample.

Protected Attributes

- size_t blockSize

  Size of the block defining a sample.

Additional Inherited Members

14.17.1 Detailed Description

template<typename OrdinalType, typename ScalarType>class Dakota::BootstrapSampler< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > >

Bootstrap sampler that is specialized to allow for the boostrapping of RealMatrix.

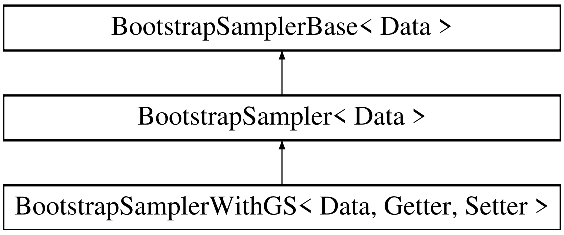
The documentation for this class was generated from the following file:

- BootstrapSampler.hpp

14.18 BootstrapSamplerBase< Data > Class Template Reference

Base class/interface for the bootstrap sampler.

Inheritance diagram for BootstrapSamplerBase< Data >:



Public Member Functions

- BootstrapSamplerBase (size_t data_size, Data orig_data)

    Constructor for the bootstrap functor base.
- virtual ~BootstrapSamplerBase ()

    Destructor.
- virtual void operator() (size_t num_samp, Data &bootstrapped_sample)=0

    Generate and store a new boostrapped sample into bootstrapped_sample.
- virtual size_t getDataSize ()

    Obatin the number of samples used in the empirical distribution.
- virtual void operator() (Data &bootstrapped_sample)

    Generate and store an dataSize out of dataSize boostrap sample.
- virtual Data operator() ()

    Return boostrapped sample.

Static Public Member Functions

- static void **set_seed** (size_t seed)

Protected Attributes

- boost::random::uniform_int_distribution sampler

    Uniform distribution to provide samples from the empirical distribution.
- const size_t dataSize

Size of the dataset defining the empirical distribution.
- Data origData

  Original data defining the empirical distribution TODO: Consider if it should be const (breaks Teuchos)

Static Protected Attributes

- static boost::random::mt19937 bootstrapRNG

  Random number generator to use for sampling.

14.18.1 Detailed Description

template< typename Data > class Dakota::BootstrapSamplerBase< Data >

Base class/interface for the bootstrap sampler.

BootstrapSamplerBase defines the minimum interface for a bootstrap sampler and handles initialization of the random variate generation used by the bootstrap. Functor is templated on the data type, but does not actually define a data member.

14.18.2 Member Data Documentation

14.18.2.1 boost::random::mt19937 bootstrapRNG [static], [protected]

Random number generator to use for sampling.

The boostrap random number generator.

Referenced by BootstrapSampler< Data >::operator()(), BootstrapSampler< Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > >::operator()(), and BootstrapSamplerWithGS< Data, Getter, Setter >::operator()().

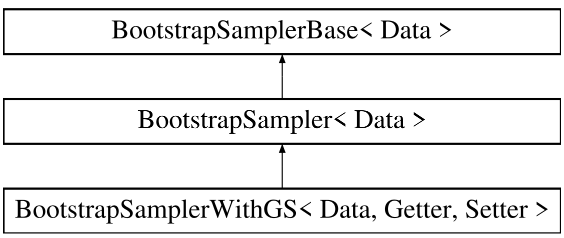
The documentation for this class was generated from the following file:

- BootstrapSampler.hpp

14.19 BootstrapSamplerWithGS< Data, Getter, Setter > Class Template Reference

A derived sampler to allow for user specification of the accessor methods.

Inheritance diagram for BootstrapSamplerWithGS< Data, Getter, Setter >:



Public Member Functions

- BootstrapSamplerWithGS (const Data &orig_data, Getter getter_method, Setter setter_method)

  Constructor with extra arguments for the accessor methods.
- virtual ~BootstrapSamplerWithGS ()

Destructor.
- virtual void operator() (size_t num_samp, Data &bootstrapped_sample)

  Generate and store a new boostrapped sample into bootstrapped_sample TODO: bounds checking.

Protected Attributes

- Getter getterMethod

  Function to obtain a single sample from a Data object. Function should take a Data object and an unsigned integer corresponding to a sample index and return the sample.
- Setter setterMethod

  Function to place a single sample into a Data object. Function should take a Data object and an unsigned integer corresponding to the sample index to set.

Additional Inherited Members

14.19.1 Detailed Description

template<typename Data, typename Getter, typename Setter>class Dakota::BootstrapSamplerWithGS< Data, Getter, Setter >

A derived sampler to allow for user specification of the accessor methods.

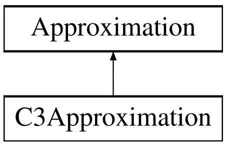
The documentation for this class was generated from the following file:

- BootstrapSampler.hpp

14.20 C3Approximation Class Reference

Derived approximation class for global basis polynomials.

Inheritance diagram for C3Approximation:



Public Member Functions

- C3Approximation ()

  default constructor
- C3Approximation (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

  standard ProblemDescDB-driven constructor
- C3Approximation (const SharedApproxData &shared_data)

  alternate constructor
- C3FnTrainData & active_ftd ()

  return the active C3FnTrainData instance in levelApprox
- C3FnTrainData & combined_ftd ()

  return combinedC3FTData
- size_t **regression_size** ()

- size_t regression_size (const SizetVector &ranks, size_t max_rank, const UShortArray &orders, unsigned short max_order)
- void **recover_function_train_ranks** (struct FunctionTrain *ft)
- void recover_function_train_orders (const std::vector< OneApproxOpts * > &a_opts)
- void **expansion_coefficient_flag** (bool coeff_flag)
- bool **expansion_coefficient_flag** () const
- void **expansion_gradient_flag** (bool grad_flag)
- bool **expansion_gradient_flag** () const
- void **compute_moments** (bool full_stats=true, bool combined_stats=false)
- void **compute_moments** (const Pecos::RealVector &x, bool full_stats=true, bool combined_stats=false)
- const RealVector & **moments** () const
- const RealVector & **expansion_moments** () const
- const RealVector & **numerical_integration_moments** () const
- const RealVector & **combined_moments** () const
- Real **moment** (size_t i) const
- void **moment** (Real mom, size_t i)
- Real **combined_moment** (size_t i) const
- void **combined_moment** (Real mom, size_t i)
- void **compute_component_effects** ()
- void **compute_total_effects** ()
- void **compute_all_sobol_indices** (size_t)
- Real **total_sobol_index** (size_t)
- Real **main_sobol_index** (size_t)
- void **sobol_iterate_apply** (void(*)(double, size_t, size_t *, void *), void *)
- Real mean ()

  return the mean of the expansion, where all active vars are random
- Real mean (const RealVector &)

  return the mean of the expansion for a given parameter vector, where a subset of the active variables are random
- const RealVector & mean_gradient ()

  return the gradient of the expansion mean
- const RealVector & mean_gradient (const RealVector &, const SizetArray &)

  return the gradient of the expansion mean
- Real variance ()

  return the variance of the expansion, where all active vars are random
- Real variance (const RealVector &)

  return the variance of the expansion for a given parameter vector, where a subset of the active variables are random
- const RealVector & **variance_gradient** ()
- const RealVector & **variance_gradient** (const RealVector &, const SizetArray &)
- Real covariance (Approximation &approx_2)

  return the covariance between two response expansions, treating all variables as random
- Real covariance (const RealVector &x, Approximation &approx_2)

  return the covariance between two response expansions, treating a subset of the variables as random
- Real **skewness** ()
- Real **kurtosis** ()
- Real **third_central** ()
- Real **fourth_central** ()
- Real combined_mean ()

  return the mean of the combined expansion, where all active vars are random
- Real combined_mean (const RealVector &)

  return the mean of the combined expansion for a given parameter vector, where a subset of the active variables are random
- Real **combined_variance** ()
- Real **combined_variance** (const RealVector &)

- Real combined_covariance (Approximation &approx_2)

    return the covariance between two combined response expansions, where all active variables are random

- Real combined_covariance (const RealVector &x, Approximation &approx_2)

    return the covariance between two combined response expansions, where a subset of the active variables are random

- Real **combined_third_central** ()
- Real **combined_fourth_central** ()
- void synchronize_surrogate_data ()

    update surrData to define aggregated data from raw data, when indicated by an active aggregated key

- void generate_synthetic_data (Pecos::SurrogateData &surr_data, const Pecos::ActiveKey &active_key, short combine_type)

    generate synthetic data for the surrogate QoI prediction corresponding to the level key preceding active key; for use in surplus estimation for new level data relative to a previous level's surrogate prediction

Protected Member Functions

- void active_model_key (const Pecos::ActiveKey &key)

    activate an approximation state based on its multi-index key

- void clear_model_keys ()

    reset initial state by removing all model keys for an approximation

- Real value (const Variables &vars)

    retrieve the approximate function value for a given parameter vector

- const RealVector & gradient (const Variables &vars)

    retrieve the approximate function gradient for a given parameter vector

- const RealSymMatrix & hessian (const Variables &vars)

    retrieve the approximate function Hessian for a given parameter vector

- bool advancement_available ()

    check if resolution advancement (e.g., order, rank) is available for this approximation instance

- void build ()

    builds the approximation from scratch

- void rebuild ()

    rebuilds the approximation incrementally

- void pop_coefficients (bool save_data)

    removes entries from end of SurrogateData::{vars,resp}Data (last points appended, or as specified in args)

- void push_coefficients ()

    restores state prior to previous pop()

- void combine_coefficients ()

    combine all level approximations into a single aggregate approximation

- void combined_to_active_coefficients (bool clear_combined=true)

    promote combined approximation into active approximation

- void clear_inactive_coefficients ()

    prune inactive coefficients following combination and promotion to active

- int min_coefficients () const

    return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions

Private Member Functions

- bool **max_rank_advancement_available** ()
- bool **max_order_advancement_available** ()
- Real **stored_value** (const RealVector &c_vars, const Pecos::ActiveKey &key)
- void **compute_derived_statistics** (C3FnTrainData &ftd, size_t num_mom, bool overwrite=false)
- void **compute_derived_statistics_av** (C3FnTrainData &ftd, size_t num_mom, bool overwrite=false)
- void check_function_gradient ()

  differentiate the ft to form its gradient, if not previously performed
- void check_function_hessian ()

  differentiate the ftg to form the ft Hessian, if not previously performed
- Real mean (C3FnTrainData &ftd)

  compute mean corresponding to the passed FT expansion
- Real mean (const RealVector &x, C3FnTrainData &ftd)

  compute mean corresponding to the passed FT expansion
- Real variance (C3FnTrainData &ftd)

  compute variance corresponding to the passed FT expansion
- Real variance (const RealVector &x, C3FnTrainData &ftd)

  compute variance corresponding to the passed FT expansion
- Real covariance (C3FnTrainData &ftd1, C3FnTrainData &ftd2)

  compute variance corresponding to the passed FT expansion
- Real covariance (const RealVector &x, C3FnTrainData &ftd1, C3FnTrainData &ftd2)

  compute variance corresponding to the passed FT expansion
- Real third_central (C3FnTrainData &ftd)

  compute 3rd central moment corresponding to the passed FT expansion
- Real fourth_central (C3FnTrainData &ftd)

  compute 4th central moment corresponding to the passed FT expansion
- Real skewness (C3FnTrainData &ftd)

  compute skewness corresponding to the passed FT expansion
- Real kurtosis (C3FnTrainData &ftd)

  compute excess kurtosis corresponding to the passed FT expansion

Private Attributes

- std::map< Pecos::ActiveKey,
  C3FnTrainData > levelApprox

  set of pointers to QoI approximation data for each model key
- std::map< Pecos::ActiveKey,
  C3FnTrainData >::iterator levApproxIter

  iterator to active levelApprox
- C3FnTrainData prevC3FTData

  the previous approximation, cached for restoration
- std::map< Pecos::ActiveKey,
  std::deque< C3FnTrainData > > poppedLevelApprox

  bookkeeping for previously evaluated FT approximations that may be restored
- C3FnTrainData combinedC3FTData

  the combined approximation, summed across model keys
- RealVector secondaryMoments

  secondary (numerical) moments: inactive
- RealVector combinedMoments

  combined moments from multilevel-multifidelity FT rollup

- bool expansionCoeffFlag

    flag indicating need to build a fn train approximation for this QoI
- bool expansionCoeffGradFlag

    flag indicating need to build a fn train gradient approx for this QoI

Additional Inherited Members

14.20.1 Detailed Description

Derived approximation class for global basis polynomials.

The PecosApproximation class provides a global approximation based on basis polynomials. This includes orthogonal polynomials used for polynomial chaos expansions and interpolation polynomials used for stochastic collocation.

14.20.2 Member Function Documentation

14.20.2.1 size_t regression_size (const SizetVector & *ranks,* size_t *max_rank,* const UShortArray & *orders,* unsigned short *max_order*)

compute the regression size (number of unknowns) for ranks per dimension and (polynomial) basis orders per dimension

References Dakota::abort_handler(), and Approximation::sharedDataRep.

14.20.2.2 void recover_function_train_orders (const std::vector< OneApproxOpts * > & *a_opts*)

returns the recovered orders, reflecting the latest CV if adapt_order

References C3Approximation::levApproxIter, SharedApproxData::numVars, and Approximation::sharedDataRep.

Referenced by C3Approximation::build().

14.20.2.3 void build ( ) [protected], [virtual]

builds the approximation from scratch

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

References Approximation::approxData, Approximation::build(), C3FnTrainData::free_all(), C3FnTrainData::function_train(), C3Approximation::levApproxIter, C3Approximation::recover_function_train_orders(), Approximation::sharedDataRep, C3Approximation::synchronize_surrogate_data(), Dakota::SZ_MAX, and Dakota::write_precision.

Referenced by C3Approximation::rebuild().

The documentation for this class was generated from the following files:

- C3Approximation.hpp
- C3Approximation.cpp

14.21 C3FnTrainData Class Reference

Handle for reference-counted pointer to C3FnTrainDataRep body.

Public Member Functions

- C3FnTrainData ()

    default constructor
- C3FnTrainData (const C3FnTrainData &ftd)

    copy constructor
- ∼C3FnTrainData ()

    destructor
- C3FnTrainData & operator= (const C3FnTrainData &ftd)

    assignment operator
- C3FnTrainData copy () const

    perform a deep copy (copy ctor and operator= use shallow copies)
- void swap (C3FnTrainData &ftd)

    swap ftdReps between two envelopes
- void free_ft ()

    free FT storage for value, gradient, and Hessian expansions
- void free_all ()

    augment free_ft() with derived functions and global sensitivities
- void ft_derived_functions_init_null ()

    initialize derived funtions pointers to NULL
- void ft_derived_functions_create (struct MultiApproxOpts ∗opts, size_t num_mom, Real round_tol)

    allocate derived funtions pointers (standard mode)
- void ft_derived_functions_create_av (struct MultiApproxOpts ∗opts, const SizetArray &rand_indices, Real round_tol)

    allocate derived funtions pointers (all variables mode)
- void ft_derived_functions_free ()

    deallocate derived funtions pointers
- struct FunctionTrain ∗ function_train ()

    get pointer to the FunctionTrain approximation
- void function_train (struct FunctionTrain ∗ft)

    set pointer to the FunctionTrain approximation
- struct FT1DArray ∗ ft_gradient ()

    get pointer to the FunctionTrain gradient
- void ft_gradient (struct FT1DArray ∗ftg)

    set pointer to the FunctionTrain gradient
- struct FT1DArray ∗ ft_hessian ()

    get pointer to the FunctionTrain Hessian
- void ft_hessian (struct FT1DArray ∗fth)

    set pointer to the FunctionTrain Hessian
- struct FTDerivedFunctions & derived_functions ()

    return reference to the FTDerivedFunctions instance
- struct C3SobolSensitivity ∗ sobol ()

    get pointer to the Sobol' indices object
- void sobol (struct C3SobolSensitivity ∗ss)

    set pointer to the Sobol' indices object
- const UShortArray & **recovered_orders** () const
- UShortArray & **recovered_orders** ()
- void **recovered_orders** (const UShortArray &ft_orders)
- const SizetVector & **recovered_ranks** () const
- SizetVector & **recovered_ranks** ()
- void **recovered_ranks** (const SizetVector &ft_ranks)
- const RealVector & **moments** () const
- RealVector & **moments** ()
- Real **moment** (size_t i) const
- void **moment** (Real mom, size_t i)

Public Attributes

- std::shared_ptr< C3FnTrainDataRep > ftdRep

    (shared) pointer to body instance

14.21.1 Detailed Description

Handle for reference-counted pointer to C3FnTrainDataRep body.

The documentation for this class was generated from the following files:

- C3FnTrainData.hpp
- C3FnTrainData.cpp

14.22 callback_data Struct Reference

Public Attributes

- double rosen_cdv_upper_bd

    upper bound value to pass through parser to callback function

14.22.1 Detailed Description

Data structure to pass application-specific values through Dakota back to the callback function, for example to convey late updates to bounds, initial points, etc., to Dakota.

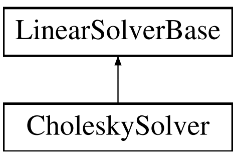
The documentation for this struct was generated from the following file:

- library_mode.cpp

14.23 CholeskySolver Class Reference

The CholeskySolver class is used to solve linear systems with a symmetric matrix with a pivoted Cholesky decomposition.

Inheritance diagram for CholeskySolver:



Public Member Functions

- CholeskySolver ()

    Constructor.
- ∼CholeskySolver ()

    Destructor.
- bool is_factorized () const override

    Query to determine if the matrix of the solver has been factored.

- void factorize (const MatrixXd &A) override

  Perform the matrix factorization for the linear solver matrix.
- void solve (const MatrixXd &A, const MatrixXd &b, MatrixXd &x) override

  Find a solution to Ax = b.
- void solve (const MatrixXd &b, MatrixXd &x) override

  Find a solution to Ax = b when A is already factorized.

Private Attributes

- std::shared_ptr< Eigen::LDLT < MatrixXd > > LDLT_Ptr

  Cached LDL^T factorization.

Additional Inherited Members

14.23.1 Detailed Description

The CholeskySolver class is used to solve linear systems with a symmetric matrix with a pivoted Cholesky decomposition.

14.23.2 Member Function Documentation

14.23.2.1 void factorize (const MatrixXd & *A*) [override], [virtual]

Perform the matrix factorization for the linear solver matrix.

Parameters

in	*A*	The incoming matrix to factorize.

Reimplemented from LinearSolverBase.

References CholeskySolver::LDLT_Ptr.

Referenced by CholeskySolver::solve().

14.23.2.2 void solve (const MatrixXd & *A*, const MatrixXd & *b*, MatrixXd & *x*) [override], [virtual]

Find a solution to Ax = b.

Parameters

in	*A*	The linear system left-hand-side matrix.
in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented from LinearSolverBase.

References CholeskySolver::factorize().

14.23.2.3 void solve (const MatrixXd & *b*, MatrixXd & *x*) [override], [virtual]

Find a solution to Ax = b when A is already factorized.

Parameters

in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented from LinearSolverBase.

References CholeskySolver::LDLT_Ptr.

The documentation for this class was generated from the following files:

- UtilLinearSolvers.hpp
- UtilLinearSolvers.cpp

14.24 COLINApplication Class Reference

Inherits Application< colin::MO_MINLP2_problem >.

Public Member Functions

- COLINApplication ()

    Default constructor. Rrequired by COLIN's ApplicationHandle creation.
- COLINApplication (Model &model)

    Constructor with Model (not presently used).
- ∼COLINApplication ()

    Destructor.
- void set_problem (Model &model)

    Helper function called after default construction to extract problem information from the Model and set it for COLIN.
- void set_blocking_synch (const bool blockingSynchFlag)

    publishes whether or not COLIN is operating synchronously
- virtual utilib::Any spawn_evaluation_impl (const utilib::Any &domain, const colin::AppRequest::request_map-_t &requests, utilib::seed_t &seed)

    Schedule one or more requests at specified domain point, returning a DAKOTA-specific evaluation tracking ID.
- virtual bool evaluation_available ()

    Check to see if there are any function values ready to be collected.
- virtual void perform_evaluation_impl (const utilib::Any &domain, const colin::AppRequest::request_map_t &requests, utilib::seed_t &seed, colin::AppResponse::response_map_t &colin_responses)

    Perform a function evaluation at t given point.
- virtual utilib::Any collect_evaluation_impl (colin::AppResponse::response_map_t &responses, utilib::seed_t &seed)

    Collect a completed evaluation from DAKOTA.
- virtual void colin_request_to_dakota_request (const utilib::Any &domain, const colin::AppRequest::request_-map_t &requests, utilib::seed_t &seed)

    Helper function to convert evaluation request data from COLIN structures to DAKOTA structures.
- virtual void dakota_response_to_colin_response (const Response &dakota_response, colin::AppResponse-::response_map_t &colin_responses)

    Gelper function to convert evaluation response data from DAKOTA structures to COLIN structures.
- virtual bool map_domain (const utilib::Any &src, utilib::Any &native, bool forward=true) const

    Map the domain point into data type desired by this application context.

Protected Attributes

- Model iteratedModel

    Shallow copy of the model on which COLIN will iterate.
- bool blockingSynch

    Flag for COLIN synchronous behavior (Pattern Search only).
- ActiveSet activeSet

    Local copy of model's active set for convenience.
- std::vector< int > requestedEvals

    Evaluations queued for asynch evaluation.
- IntResponseMap dakota_responses

    eval_id to response mapping to cache completed jobs.

14.24.1 Detailed Description

COLINApplication is a DAKOTA class that is derived from COLIN's Application hierarchy. It redefines a variety of virtual COLIN functions to use the corresponding DAKOTA functions. This is a more flexible algorithm library interfacing approach than can be obtained with the function pointer approaches used by NPSOLOptimizer and SNLLOptimizer.

14.24.2 Member Function Documentation

14.24.2.1 void set_problem (Model & *model*)

Helper function called after default construction to extract problem information from the Model and set it for COLIN.

Set variable bounds and linear and nonlinear constraints. This avoids using probDescDB, so it is called by both the standard and the on-the-fly COLINOptimizer constructors.

References Response::active_set(), COLINApplication::activeSet, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Dakota::copy_data_partial(), Model::current_response(), Model::cv(), Model::discrete_int_lower_bounds(), Model::discrete_int_sets(), Model::discrete_int_upper_bounds(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Model::div(), Model::drv(), Model::dsv(), Dakota::get_nonlinear_bounds(), COLINApplication::iteratedModel, Model::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_targets(), Model::linear_ineq_constraint_coeffs(), Model::linear_ineq_constraint_lower_bounds(), Model::linear_ineq_constraint_upper_bounds(), Model::num_linear_eq_constraints(), Model::num_linear_ineq_constraints(), Model::num_primary_fns(), Model::num_secondary_fns(), and Model::primary_response_fn_sense().

Referenced by COLINApplication::COLINApplication().

14.24.2.2 utilib::Any spawn_evaluation_impl (const utilib::Any & *domain,* const colin::AppRequest::request_map_t & *requests,* utilib::seed_t & *seed*) [virtual]

Schedule one or more requests at specified domain point, returning a DAKOTA-specific evaluation tracking ID.

Schedule one or more requests at specified domain point, returning a DAKOTA-specific evaluation tracking ID. This is only called by COLIN's concurrent evaluator, which is only instantiated when the Model supports asynch evals. The domain point is guaranteed to be compatible with data type specified by map_domain(...)

References COLINApplication::colin_request_to_dakota_request(), Model::evaluate_nowait(), Model::evaluation_id(), and COLINApplication::iteratedModel.

14.24.2.3 bool evaluation_available ( ) [virtual]

Check to see if there are any function values ready to be collected.

Check to see if any asynchronous evaluations have finished. This is only called by COLIN's concurrent evaluator, which is only instantiated when the Model supports asynch evals.

References COLINApplication::blockingSynch, COLINApplication::dakota_responses, COLINApplication::iterated-Model, Model::synchronize(), and Model::synchronize_nowait().

14.24.2.4 void perform_evaluation_impl (const utilib::Any & *domain,* const colin::AppRequest::request_map_t & *requests,* utilib::seed_t & *seed,* colin::AppResponse::response_map_t & *colin_responses*) [virtual]

Perform a function evaluation at t given point.

Perform an evaluation at a specified domain point. Wait for and return the response. This is only called by COLIN's serial evaluator, which is only instantiated when the Model does not support asynch evals. The domain point is guaranteed to be compatible with data type specified by map_domain(...)

References COLINApplication::colin_request_to_dakota_request(), Model::current_response(), COLINApplication-::dakota_response_to_colin_response(), Model::evaluate(), and COLINApplication::iteratedModel.

14.24.2.5 utilib::Any collect_evaluation_impl (colin::AppResponse::response_map_t & *colin_responses,* utilib::seed_t & *seed*) [virtual]

Collect a completed evaluation from DAKOTA.

Collect the next completed evaluation from DAKOTA. Always returns the evalid of the response returned.

References COLINApplication::dakota_response_to_colin_response(), and COLINApplication::dakota_responses.

14.24.2.6 void colin_request_to_dakota_request (const utilib::Any & *domain,* const colin::AppRequest::request_map_t & *requests,* utilib::seed_t & *seed*) [virtual]

Helper function to convert evaluation request data from COLIN structures to DAKOTA structures.

Map COLIN info requests to DAKOTA objectives and constraints.

References Model::continuous_variables(), Model::discrete_int_sets(), Model::discrete_int_variable(), Model-::discrete_real_variable(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete-_set_string_values(), Model::discrete_string_variable(), Model::div(), Model::drv(), Model::dsv(), COLINApplication-::iteratedModel, Model::response_size(), and Dakota::set_index_to_value().

Referenced by COLINApplication::perform_evaluation_impl(), and COLINApplication::spawn_evaluation_impl().

14.24.2.7 void dakota_response_to_colin_response (const Response & *dakota_response,* colin::AppResponse::response_map_t & *colin_responses*) [virtual]

Gelper function to convert evaluation response data from DAKOTA structures to COLIN structures.

Map DAKOTA objective and constraint values to COLIN response.

References Response::active_set_request_vector(), and Response::function_value().

Referenced by COLINApplication::collect_evaluation_impl(), and COLINApplication::perform_evaluation_impl().

14.24.2.8 bool map_domain (const utilib::Any & *src,* utilib::Any & *native,* bool *forward* = true) const [virtual]

Map the domain point into data type desired by this application context.

Map the domain point into data type desired by this application context (utilib::MixedIntVars). This data type can be exposed from the Any &domain presented to spawn and collect.

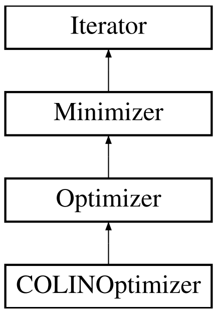
The documentation for this class was generated from the following files:

- COLINApplication.hpp
- COLINApplication.cpp

14.25 COLINOptimizer Class Reference

Wrapper class for optimizers defined using COLIN.

Inheritance diagram for COLINOptimizer:



Public Member Functions

- COLINOptimizer (ProblemDescDB &problem_db, Model &model)

    standard constructor
- COLINOptimizer (const String &method_name, Model &model, int seed, size_t max_iter, size_t max_eval)

    alternate constructor for on-the-fly instantiations
- COLINOptimizer (const String &method_name, Model &model)

    alternate constructor for Iterator instantiations by name
- ∼COLINOptimizer ()

    destructor
- void reset ()

    clears internal optimizer state
- void core_run ()

    iterates the COLIN solver to determine the optimal solution
- bool returns_multiple_points () const

    some COLIN methods can return multiple points

Protected Member Functions

- void solver_setup (unsigned short method_name)

    convenience function for setting up the particular COLIN solver and appropriate Application
- void set_rng (int seed)

    sets up the random number generator for stochastic methods
- void set_solver_parameters ()

    sets construct-time options for specific methods based on user specifications, including calling method-specific set functions
- void post_run (std::ostream &s)

    Get the final set of points from the solver Look up responses and sort, first according to constraint violation, then according to function value.
- std::pair< bool, bool > colin_cache_lookup (const colin::AppResponse &colinResponse, Response &tmpResponseHolder)

Retrieve response from Colin AppResponse, return pair indicating success for <objective, constraints>

- double constraint_violation (const Response &tmpResponseHolder)

    Compute constraint violation, based on nonlinear constraints in iteratedModel and provided Response data.

Protected Attributes

- short solverType

    COLIN solver sub-type as enumerated in COLINOptimizer.cpp.
- colin::SolverHandle colinSolver

    handle to the COLIN solver
- std::pair
  < colin::ApplicationHandle,
  COLINApplication ∗ > colinProblem

    handle and pointer to the COLINApplication object
- colin::EvaluationManager_Base ∗ colinEvalMgr

    pointer to the COLIN evalutaion manager object
- utilib::RNG ∗ rng

    random number generator pointer
- bool blockingSynch

    the `synchronization` setting: true if `blocking`, false if `nonblocking`
- Real constraint_penalty

    Buffer to hold problem constraint_penalty parameter.
- bool constant_penalty

    Buffer to hold problem constant_penalty parameter.

Additional Inherited Members

14.25.1 Detailed Description

Wrapper class for optimizers defined using COLIN.

The COLINOptimizer class wraps COLIN, a Sandia-developed C++ optimization interface library. A variety of COLIN optimizers are defined in COLIN and its associated libraries, including SCOLIB which contains the optimization components from the old COLINY (formerly SGOPT) library. COLIN contains optimizers such as genetic algorithms, pattern search methods, and other nongradient-based techniques. COLINOptimizer uses a COLINApplication object to perform the function evaluations.

The user input mappings are as follows: `max_iterations`, `max_function_evaluations`, `convergence_tolerance`, and `solution_accuracy` are mapped into COLIN's `max_iterations`, `max_function_evaluations_this_trial`, `function_value_tolerance`, `sufficient_objective_value` properties. An `outputLevel` is mapped to COLIN's `output_level` property and a setting of `debug` activates output of method initialization and sets the COLIN `debug` attribute to 10000 for the DEBUG output level. Refer to [Hart, W.E., 2006] for additional information on COLIN objects and controls.

14.25.2 Constructor & Destructor Documentation

14.25.2.1 COLINOptimizer (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

Standard constructor.

References ProblemDescDB::get_int(), ProblemDescDB::get_ushort(), Iterator::probDescDB, COLINOptimizer::set_rng(), COLINOptimizer::set_solver_parameters(), and COLINOptimizer::solver_setup().

14.25.2.2 COLINOptimizer (const String & *method_name,* Model & *model,* int *seed,* size_t *max_iter,* size_t *max_eval*)

alternate constructor for on-the-fly instantiations

Alternate constructor for on-the-fly instantiations.

References Iterator::maxFunctionEvals, Iterator::maxIterations, Iterator::method_string_to_enum(), COLINOptimizer::set_rng(), COLINOptimizer::set_solver_parameters(), and COLINOptimizer::solver_setup().

14.25.2.3 COLINOptimizer (const String & *method_name,* Model & *model*)

alternate constructor for Iterator instantiations by name

Alternate constructor for Iterator instantiations by name.

References Iterator::method_string_to_enum(), COLINOptimizer::set_solver_parameters(), and COLINOptimizer::solver_setup().

14.25.3 Member Function Documentation

14.25.3.1 void core_run ( ) [virtual]

iterates the COLIN solver to determine the optimal solution

core_run redefines the Optimizer virtual function to perform the optimization using COLIN. It first sets up the problem data, then executes optimize() on the COLIN solver and finally catalogues the results.

Reimplemented from Iterator.

References Dakota::abort_handler(), Model::asynch_flag(), COLINOptimizer::blockingSynch, COLINOptimizer::colinEvalMgr, COLINOptimizer::colinProblem, COLINOptimizer::colinSolver, COLINOptimizer::constant_penalty, COLINOptimizer::constraint_penalty, Model::continuous_variables(), Model::discrete_int_sets(), Model::discrete_int_variables(), Model::discrete_real_variables(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Model::discrete_string_variables(), Model::evaluation_capacity(), Iterator::iteratedModel, Minimizer::numDiscreteIntVars, Minimizer::numDiscreteRealVars, Minimizer::numDiscreteStringVars, Iterator::outputLevel, Dakota::set_value_to_index(), and COLINOptimizer::solverType.

14.25.3.2 bool returns_multiple_points ( ) const [virtual]

some COLIN methods can return multiple points

Designate which solvers can return multiple final points.

Reimplemented from Iterator.

References COLINOptimizer::solverType.

14.25.3.3 void solver_setup (unsigned short *method_name*) [protected]

convenience function for setting up the particular COLIN solver and appropriate Application

This convenience function is called by the constructors in order to instantiate the solver.

References COLINOptimizer::colinProblem, COLINOptimizer::colinSolver, COLINOptimizer::constant_penalty, COLINOptimizer::constraint_penalty, ProblemDescDB::get_string(), Iterator::method_enum_to_string(), Iterator::probDescDB, and COLINOptimizer::solverType.

Referenced by COLINOptimizer::COLINOptimizer().

14.25.3.4 void set_rng (int *seed*) [protected]

sets up the random number generator for stochastic methods

Instantiate random number generator (RNG).

References COLINOptimizer::colinSolver, and COLINOptimizer::rng.

Referenced by COLINOptimizer::COLINOptimizer().

14.25.3.5 void set_solver_parameters ( ) [protected]

sets construct-time options for specific methods based on user specifications, including calling method-specific set functions

Sets solver properties based on user specifications. Called at construction time.

References Model::asynch_flag(), COLINOptimizer::blockingSynch, COLINOptimizer::colinSolver, COLINOptimizer::constant_penalty, COLINOptimizer::constraint_penalty, Iterator::convergenceTol, ProblemDescDB::get_bool(), ProblemDescDB::get_int(), ProblemDescDB::get_real(), ProblemDescDB::get_sa(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), ProblemDescDB::is_null(), Iterator::iteratedModel, Iterator::maxEvalConcurrency, Iterator::maxFunctionEvals, Iterator::maxIterations, Minimizer::numContinuousVars, Iterator::outputLevel, Iterator::probDescDB, and COLINOptimizer::solverType.

Referenced by COLINOptimizer::COLINOptimizer().

14.25.3.6 void post_run (std::ostream & *s*) [protected], [virtual]

Get the final set of points from the solver Look up responses and sort, first according to constraint violation, then according to function value.

Supplement Optimizer::post_run to first retrieve points from the Colin cache (or possibly the Dakota DB) and rank them. When complete, this function will populate bestVariablesArray and bestResponsesArray with iterator-space data, that is, in the context of the solver, leaving any further untransformation to Optimizer.

Reimplemented from Iterator.

References Iterator::bestResponseArray, Iterator::bestVariablesArray, COLINOptimizer::colin_cache_lookup(), COLINOptimizer::colinProblem, COLINOptimizer::colinSolver, COLINOptimizer::constraint_violation(), Variables::continuous_variables(), Response::copy(), Variables::copy(), Model::current_response(), Model::current_variables(), Model::discrete_int_sets(), Variables::discrete_int_variable(), Variables::discrete_real_variable(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Variables::discrete_string_variable(), Response::function_values(), Iterator::iteratedModel, Optimizer::localObjectiveRecast, Minimizer::numDiscreteIntVars, Minimizer::numDiscreteRealVars, Minimizer::numDiscreteStringVars, Iterator::numFinalSolutions, Minimizer::numNonlinearConstraints, Optimizer::numObjectiveFns, Minimizer::numUserPrimaryFns, Minimizer::objective(), Optimizer::post_run(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), Minimizer::resize_best_resp_array(), Minimizer::resize_best_vars_array(), Dakota::set_index_to_value(), COLINOptimizer::solverType, and Model::subordinate_model().

14.25.3.7 std::pair< bool, bool > colin_cache_lookup (const colin::AppResponse & *colinResponse,* Response & *tmpResponseHolder*) [protected]

Retrieve response from Colin AppResponse, return pair indicating success for <objective, constraints>

Encapsulated Colin Cache response extraction, which will ultimately become the default lookup. Might want to return separate vectors of function values and constraints for use in the sort, but not for now (least change). Return true if not needed or successful lookup.

References Response::function_value(), Minimizer::numNonlinearConstraints, and Optimizer::numObjectiveFns.

Referenced by COLINOptimizer::post_run().

14.25.3.8 double constraint_violation (const Response & *tmpResponseHolder*) [protected]

Compute constraint violation, based on nonlinear constraints in iteratedModel and provided Response data.

BMA TODO: incorporate constraint tolerance, possibly via elevating SurrBasedMinimizer::constraint_violation(). Always use iteratedModel to get the constraints; they are in the right space.

References Response::function_values(), Iterator::iteratedModel, Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), and Minimizer::numIterPrimaryFns.

Referenced by COLINOptimizer::post_run().

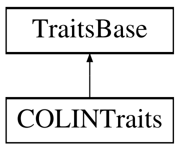
The documentation for this class was generated from the following files:

- COLINOptimizer.hpp
- COLINOptimizer.cpp

14.26 COLINTraits Class Reference

A version of TraitsBase specialized for COLIN optimizers.

Inheritance diagram for COLINTraits:



Public Member Functions

- COLINTraits ()

    default constructor
- virtual ∼COLINTraits ()

    destructor
- virtual bool is_derived ()

    A temporary query used in the refactor.
- bool supports_continuous_variables ()

    Return the flag indicating whether method supports continuous variables.
- bool supports_nonlinear_equality ()

    Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

    Return the flag indicating whether method supports nonlinear inequalities.
- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()

    Return the format used for nonlinear inequality constraints.

14.26.1 Detailed Description

A version of TraitsBase specialized for COLIN optimizers.

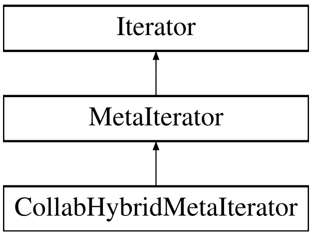
The documentation for this class was generated from the following file:

- COLINOptimizer.hpp

14.27 CollabHybridMetaIterator Class Reference

Meta-iterator for hybrid iteration using multiple collaborating optimization and nonlinear least squares methods.

Inheritance diagram for CollabHybridMetaIterator:



Public Member Functions

- CollabHybridMetaIterator (ProblemDescDB &problem_db)

  standard constructor
- CollabHybridMetaIterator (ProblemDescDB &problem_db, Model &model)

  alternate constructor
- ∼CollabHybridMetaIterator ()

  destructor

Protected Member Functions

- void core_run ()

  Performs the collaborative hybrid iteration.
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- IntIntPair estimate_partition_bounds ()

  estimate the minimum and maximum partition sizes that can be utilized by this Iterator
- const Variables & variables_results () const

  return the final solution from the collaborative iteration (variables)
- const Response & response_results () const

  return the final solution from the collaborative iteration (response)

Private Attributes

- String hybridCollabType

  abo or hops
- StringArray methodStrings

  the list of method pointer or method name identifiers
- StringArray modelStrings

  the list of model pointer identifiers for method identification by name
- bool lightwtMethodCtor

  use of lightweight Iterator construction by name
- bool singlePassedModel

use of constructor that enforces use of a single passed Model

- IteratorArray selectedIterators

  the set of iterators, one for each entry in methodStrings
- ModelArray selectedModels

  the set of models, one for each iterator
- Variables bestVariables

  best variables found in collaborative iteration
- Response bestResponse

  best response found in collaborative iteration

Additional Inherited Members

14.27.1 Detailed Description

Meta-iterator for hybrid iteration using multiple collaborating optimization and nonlinear least squares methods.

This meta-iterator has two approaches to hybrid iteration: (1) agent-based using the ABO framework; (2) nonagent-based using the HOPSPACK framework.

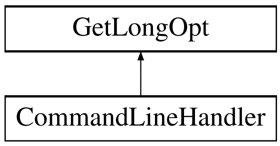
The documentation for this class was generated from the following files:

- CollabHybridMetaIterator.hpp
- CollabHybridMetaIterator.cpp

14.28 CommandLineHandler Class Reference

Utility class for managing command line inputs to DAKOTA.

Inheritance diagram for CommandLineHandler:



Public Member Functions

- CommandLineHandler ()

  default constructor, requires check_usage() call for parsing
- CommandLineHandler (int argc, char ∗∗argv, int world_rank)

  constructor with parsing
- ∼CommandLineHandler ()

  destructor
- void check_usage (int argc, char ∗∗argv)

  Verifies that DAKOTA is called with the correct command usage. Prints a descriptive message and exits the program if incorrect.
- int read_restart_evals () const

  Returns the number of evaluations to be read from the restart file (as specified on the DAKOTA command line) as an integer instead of a const char∗.
- void usage (std::ostream &outfile=Cout) const

  Print usage information to outfile, conditionally on rank.

Private Member Functions

- void initialize_options ()

  enrolls the supported command line inputs.
- void output_helper (const std::string &message, std::ostream &os) const

  output only on Dakota worldRank 0 if possible

Private Attributes

- int worldRank

  Rank of this process within Dakota's allocation; manages conditional output.

Additional Inherited Members

14.28.1 Detailed Description

Utility class for managing command line inputs to DAKOTA.

CommandLineHandler provides additional functionality that is specific to DAKOTA's needs for the definition and parsing of command line options. Inheritance is used to allow the class to have all the functionality of the base class, GetLongOpt.

14.28.2 Member Function Documentation

14.28.2.1 void output_helper (const std::string & *message,* std::ostream & *os*) const [private]

output only on Dakota worldRank 0 if possible

When there is a valid ParallelLibrary, output only on rank 0

References CommandLineHandler::worldRank.

Referenced by CommandLineHandler::check_usage().

The documentation for this class was generated from the following files:

- CommandLineHandler.hpp
- CommandLineHandler.cpp

14.29 CommandShell Class Reference

Utility class which defines convenience operators for spawning processes with system calls.

Public Member Functions

- CommandShell ()

  constructor
- ∼CommandShell ()

  destructor
- CommandShell & operator<< (const char ∗cmd)

  appends cmd to sysCommand
- CommandShell & operator<< (const std::string &cmd)

  convenient operator: appends string to the commandString to be executed

- CommandShell & operator<< (CommandShell &(∗f)(CommandShell &))

    allows passing of the flush function to the shell using <<
- CommandShell & flush ()

    "flushes" the shell; i.e. executes the sysCommand
- void asynch_flag (const bool flag)

    set the asynchFlag
- bool asynch_flag () const

    get the asynchFlag
- void suppress_output_flag (const bool flag)

    set the suppressOutputFlag
- bool suppress_output_flag () const

    get the suppressOutputFlag

Private Attributes

- std::string sysCommand

    The command string that is constructed through one or more << insertions and then executed by flush.
- bool asynchFlag

    flags nonblocking operation (background system calls)
- bool suppressOutputFlag

    flags suppression of shell output (no command echo)

14.29.1 Detailed Description

Utility class which defines convenience operators for spawning processes with system calls.

The CommandShell class wraps the C system() utility and defines convenience operators for building a command string and then passing it to the shell.

14.29.2 Member Function Documentation

14.29.2.1 CommandShell & operator<< (const char ∗ *cmd*) [inline]

appends cmd to sysCommand

convenient operator: appends string to the commandString to be executed

References CommandShell::sysCommand.

14.29.2.2 CommandShell & operator<< (CommandShell &(∗)(CommandShell &) *f*) [inline]

allows passing of the flush function to the shell using <<

convenience operator: allows passing of the flush func to the shell via <<

14.29.2.3 CommandShell & flush ( )

"flushes" the shell; i.e. executes the sysCommand

Executes the sysCommand by passing it to system(). Appends an "&" if asynchFlag is set (background system call) and echos the sysCommand to Cout if suppressOutputFlag is not set.

References Dakota::abort_handler(), CommandShell::asynchFlag, CommandShell::suppressOutputFlag, and CommandShell::sysCommand.

Referenced by Dakota::flush().

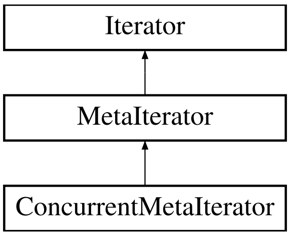
The documentation for this class was generated from the following files:

- CommandShell.hpp
- CommandShell.cpp

14.30 ConcurrentMetaIterator Class Reference

Meta-iterator for multi-start iteration or pareto set optimization.

Inheritance diagram for ConcurrentMetaIterator:



Public Member Functions

- ConcurrentMetaIterator (ProblemDescDB &problem_db)

  standard constructor
- ConcurrentMetaIterator (ProblemDescDB &problem_db, Model &model)

  alternate constructor
- ∼ConcurrentMetaIterator ()

  destructor

Protected Member Functions

- void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()

  Performs the concurrent iteration by executing selectedIterator on iteratedModel multiple times in parallel for different parameter sets.
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final iterator results
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- IntIntPair estimate_partition_bounds ()

  estimate the minimum and maximum partition sizes that can be utilized by this Iterator
- void initialize_iterator (int job_index)

  used by IteratorScheduler to set the starting data for a run
- void pack_parameters_buffer (MPIPackBuffer &send_buffer, int job_index)

used by IteratorScheduler to pack starting data for an iterator run

- void unpack_parameters_initialize (MPIUnpackBuffer &recv_buffer, int job_index)

  used by IteratorScheduler to unpack starting data and initialize an iterator run

- void pack_results_buffer (MPIPackBuffer &send_buffer, int job_index)

  used by IteratorScheduler to pack results data from an iterator run

- void unpack_results_buffer (MPIUnpackBuffer &recv_buffer, int job_index)

  used by IteratorScheduler to unpack results data from an iterator run

- void update_local_results (int job_index)

  used by IteratorScheduler to update local results arrays

- const Model & algorithm_space_model () const

  return the result of any recasting or surrogate model recursion layered on top of iteratedModel by the derived Iterator ctor chain

- virtual void declare_sources ()

  Declare sources to the evaluations database.

Private Member Functions

- void initialize_iterator (const RealVector &param_set)

  called by unpack_parameters_initialize(MPIUnpackBuffer) and initialize_iterator(int) to update iteratedModel and selectedIterator

- void initialize_model ()

  initialize the iterated Model prior to Iterator instantiation and define param_set_len

Private Attributes

- Iterator selectedIterator

  the iterator selected for concurrent iteration

- RealVector initialPt

  the initial continuous variables for restoring the starting point in the Pareto set minimization

- RealVectorArray parameterSets

  an array of parameter set vectors (either multistart variable sets or pareto multi-objective/least squares weighting sets) to be performed.

- int paramSetLen

  length of each of the parameter sets associated with an iterator job (number of continuous variables for MULTI_START, number of objective fns for PARETO_SET)

- int numRandomJobs

  number of randomly-generated parameter sets to evaluate

- int randomSeed

  seed for random number generator for random samples

- PRPArray prpResults

  1-d array of ParamResponsePair results corresponding to numIteratorJobs

Friends

- class IteratorScheduler

  protect scheduler callback functions from general access

Additional Inherited Members

14.30.1 Detailed Description

Meta-iterator for multi-start iteration or pareto set optimization.

This meta-iterator maintains two concurrent iterator capabilities. First, a general capability for running an iterator multiple times from different starting points is provided (often used for multi-start optimization, but not restricted to optimization). Second, a simple capability for mapping the "pareto frontier" (the set of optimal solutions in multiobjective formulations) is provided. This pareto set is mapped through running an optimizer multiple times for different sets of multiobjective weightings.

14.30.2 Member Function Documentation

14.30.2.1 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Iterator.

References Analyzer::all_samples(), Iterator::all_samples(), ParallelLibrary::bcast_hs(), Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Dakota::copy_data(), Model::estimate_message_lengths(), ConcurrentMetaIterator::initialPt, Iterator::iteratedModel, IteratorScheduler::iterator_message_lengths(), IteratorScheduler::iteratorCommRank, IteratorScheduler::iteratorScheduling, IteratorScheduler::iteratorServerId, MetaIterator::iterSched, IteratorScheduler::lead_rank(), Model::message_lengths(), Iterator::methodName, Iterator::methodPCIter, IteratorScheduler::miPLIndex, IteratorScheduler::numIteratorJobs, IteratorScheduler::numIteratorServers, ConcurrentMetaIterator::numRandomJobs, Iterator::parallelLib, ConcurrentMetaIterator::parameterSets, ConcurrentMetaIterator::paramSetLen, ConcurrentMetaIterator::prpResults, ConcurrentMetaIterator::randomSeed, and MPIPackBuffer::size().

14.30.2.2 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Iterator.

References ResultsManager::active(), ResultsManager::allocate_matrix(), Variables::continuous_variables(), Variables::discrete_int_variables(), Variables::discrete_real_variables(), Variables::discrete_string_variables(), ParamResponsePair::eval_id(), ResultsManager::insert_into(), Iterator::methodName, ConcurrentMetaIterator::parameterSets, ConcurrentMetaIterator::paramSetLen, ConcurrentMetaIterator::prpResults, ParamResponsePair::response(), Iterator::resultsDB, Iterator::run_identifier(), ParamResponsePair::variables(), and Response::write_tabular().

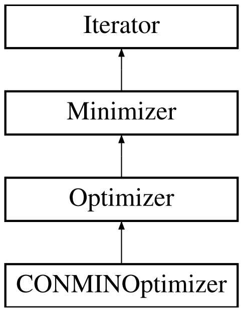
The documentation for this class was generated from the following files:

- ConcurrentMetaIterator.hpp
- ConcurrentMetaIterator.cpp

14.31 CONMINOptimizer Class Reference

Wrapper class for the CONMIN optimization library.

Inheritance diagram for CONMINOptimizer:



Public Member Functions

- CONMINOptimizer (ProblemDescDB &problem_db, Model &model)

    standard constructor
- CONMINOptimizer (const String &method_string, Model &model)

    alternate constructor; construct without ProblemDescDB
- ∼CONMINOptimizer ()

    destructor
- void core_run ()

    core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Protected Member Functions

- void initialize_run ()

    utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
- void check_sub_iterator_conflict ()

    detect any conflicts due to recursive use of the same Fortran solver

Private Member Functions

- void initialize ()

    Shared constructor code.
- void allocate_workspace ()

    Allocates workspace for the optimizer.
- void deallocate_workspace ()

    Releases workspace memory.
- void allocate_constraints ()

    Allocates constraint mappings.

Private Attributes

- int conminInfo

    INFO from CONMIN manual.
- int printControl

IPRINT from CONMIN manual (controls output verbosity)
- Real objFnValue

  value of the objective function passed to CONMIN
- RealVector constraintValues

  array of nonlinear constraint values passed to CONMIN
- int numConminNlnConstr

  total number of nonlinear constraints seen by CONMIN
- int numConminLinConstr

  total number of linear constraints seen by CONMIN
- int numConminConstr

  total number of linear and nonlinear constraints seen by CONMIN
- int N1

  Size variable for CONMIN arrays. See CONMIN manual.
- int N2

  Size variable for CONMIN arrays. See CONMIN manual.
- int N3

  Size variable for CONMIN arrays. See CONMIN manual.
- int N4

  Size variable for CONMIN arrays. See CONMIN manual.
- int N5

  Size variable for CONMIN arrays. See CONMIN manual.
- int NFDG

  Finite difference flag.
- int IPRINT

  Flag to control amount of output data.
- int ITMAX

  Flag to specify the maximum number of iterations.
- double FDCH

  Relative finite difference step size.
- double FDCHM

  Absolute finite difference step size.
- double CT

  Constraint thickness parameter.
- double CTMIN

  Minimum absolute value of CT used during optimization.
- double CTL

  Constraint thickness parameter for linear and side constraints.
- double CTLMIN

  Minimum value of CTL used during optimization.
- double DELFUN

  Relative convergence criterion threshold.
- double DABFUN

  Absolute convergence criterion threshold.
- double * conminDesVars

  Array of design variables used by CONMIN (length N1 = numdv+2)
- double * conminLowerBnds

  Array of lower bounds used by CONMIN (length N1 = numdv+2)
- double * conminUpperBnds

  Array of upper bounds used by CONMIN (length N1 = numdv+2)
- double * S

  Internal CONMIN array.

- double ∗ G1

  Internal CONMIN array.
- double ∗ G2

  Internal CONMIN array.
- double ∗ B

  Internal CONMIN array.
- double ∗ C

  Internal CONMIN array.
- int ∗ MS1

  Internal CONMIN array.
- double ∗ SCAL

  Internal CONMIN array.
- double ∗ DF

  Internal CONMIN array.
- double ∗ A

  Internal CONMIN array.
- int ∗ ISC

  Internal CONMIN array.
- int ∗ IC

  Internal CONMIN array.

Additional Inherited Members

14.31.1 Detailed Description

Wrapper class for the CONMIN optimization library.

The CONMINOptimizer class provides a wrapper for CONMIN, a Public-domain Fortran 77 optimization library written by Gary Vanderplaats under contract to NASA Ames Research Center. The CONMIN User's Manual is contained in NASA Technical Memorandum X-62282, 1978. CONMIN uses a reverse communication mode, which avoids the static member function issues that arise with function pointer designs (see NPSOLOptimizer and SNLL-Optimizer).

The user input mappings are as follows: `max_iterations` is mapped into CONMIN's `ITMAX` parameter, `max_function_evaluations` is implemented directly in the core_run() loop since there is no CONMIN parameter equivalent, `convergence_tolerance` is mapped into CONMIN's `DELFUN` and `DABFUN` parameters, `output` verbosity is mapped into CONMIN's `IPRINT` parameter (verbose: `IPRINT` = 4; quiet: `IPRINT` = 2), gradient mode is mapped into CONMIN's `NFDG` parameter, and finite difference step size is mapped into CONMIN's `FDCH` and `FDCHM` parameters. Refer to [Vanderplaats, 1978] for additional information on CONMIN parameters.

14.31.2 Member Function Documentation

14.31.2.1 void core_run ( ) `[virtual]`

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References CONMINOptimizer::A, Iterator::activeSet, CONMINOptimizer::B, Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::bigRealBoundSize, CONMINOptimizer::C, CONMINOptimizer::conminDesVars, CONMINOptimizer::conminInfo, CONMINOptimizer::conminLowerBnds, CONMINOptimizer::conminUpperBnds, Optimizer::constraintMapIndices, Optimizer::constraintMapMultipliers, Optimizer::constraintMapOffsets, CONMINOptimizer::constraintValues, Model::continuous_variables(), Dakota::copy_data(), CONMINOptimizer::CT, CONMINOptimizer::CTL, CONMINOptimizer::CTLMIN, CONMINOptimizer::CTMIN, Model::current_response(), CONMINOptimizer::DABFUN, CONMINOptimizer::deallocate_workspace(), CONMINOptimizer::DELFUN, CONMINOptimizer::DF, Model::evaluate(), CONMINOptimizer::FDCH, CONMINOptimizer::FDCHM, Response::function_gradients(), Response::function_values(), CONMINOptimizer::G1, CONMINOptimizer::G2, Model::gradient_type(), CONMINOptimizer::IC, CONMINOptimizer::IPRINT, CONMINOptimizer::ISC, Iterator::iteratedModel, CONMINOptimizer::ITMAX, Model::linear_eq_constraint_coeffs(), Model::linear_ineq_constraint_coeffs(), Optimizer::localObjectiveRecast, Iterator::maxFunctionEvals, CONMINOptimizer::MS1, CONMINOptimizer::N1, CONMINOptimizer::N2, CONMINOptimizer::N3, CONMINOptimizer::N4, CONMINOptimizer::N5, CONMINOptimizer::NFDG, Model::num_linear_eq_constraints(), Model::num_linear_ineq_constraints(), CONMINOptimizer::numConminConstr, CONMINOptimizer::numConminNlnConstr, Minimizer::numContinuousVars, Optimizer::numObjectiveFns, Minimizer::numUserPrimaryFns, CONMINOptimizer::objFnValue, Iterator::outputLevel, Model::primary_response_fn_sense(), ActiveSet::request_value(), ActiveSet::request_values(), CONMINOptimizer::S, CONMINOptimizer::SCAL, Minimizer::speculativeFlag, and Minimizer::vendorNumericalGradFlag.

14.31.2.2 void initialize_run ( ) [protected], [virtual]

utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers

Perform initialization phases of run sequence, like allocating memory and setting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's initialize_run(), typically *before* performing its own implementation steps.

Reimplemented from Iterator.

References CONMINOptimizer::allocate_constraints(), CONMINOptimizer::allocate_workspace(), CONMINOptimizer::conminDesVars, CONMINOptimizer::conminLowerBnds, CONMINOptimizer::conminUpperBnds, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), CONMINOptimizer::IC, Optimizer::initialize_run(), CONMINOptimizer::ISC, Iterator::iteratedModel, CONMINOptimizer::N1, CONMINOptimizer::numConminConstr, and Minimizer::numContinuousVars.

14.31.2.3 void check_sub_iterator_conflict ( ) [protected], [virtual]

detect any conflicts due to recursive use of the same Fortran solver

This is used to avoid clashes in state between non-object-oriented (i.e., F77, C) iterator executions, when such iterators could potentially be executing simultaneously (e.g., nested execution). It is not an issue (and a used method is not reported) in cases where a helper execution is completed before a lower level one could be initiated; an example of this is DIRECT for maximization of expected improvement: the EIF maximization is completed before a new point evaluation (which could include nested iteration) is performed.

Reimplemented from Iterator.

References Iterator::is_null(), Iterator::iteratedModel, Iterator::method_name(), Iterator::method_recourse(), Model::subordinate_iterator(), Model::subordinate_models(), and Iterator::uses_method().

14.31.3 Member Data Documentation

14.31.3.1 int conminInfo [private]

INFO from CONMIN manual.

Information requested by CONMIN: 1 = evaluate objective and constraints, 2 = evaluate gradients of objective and constraints.

Referenced by CONMINOptimizer::core_run(), and CONMINOptimizer::initialize().

14.31.3.2 int printControl [private]

IPRINT from CONMIN manual (controls output verbosity)

Values range from 0 (nothing) to 4 (most output). 0 = nothing, 1 = initial and final function information, 2 = all of #1 plus function value and design vars at each iteration, 3 = all of #2 plus constraint values and direction vectors, 4 = all of #3 plus gradients of the objective function and constraints, 5 = all of #4 plus proposed design vector, plus objective and constraint functions from the 1-D search

Referenced by CONMINOptimizer::initialize().

14.31.3.3 RealVector constraintValues [private]

array of nonlinear constraint values passed to CONMIN

This array must be of nonzero length and must contain only one-sided inequality constraints which are $<=$ 0 (which requires a transformation from 2-sided inequalities and equalities).

Referenced by CONMINOptimizer::allocate_workspace(), and CONMINOptimizer::core_run().

14.31.3.4 int N1 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N1 = number of variables + 2

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::initialize_run().

14.31.3.5 int N2 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N2 = number of constraints + 2$*$(number of variables)

Referenced by CONMINOptimizer::allocate_workspace(), and CONMINOptimizer::core_run().

14.31.3.6 int N3 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N3 = Maximum possible number of active constraints.

Referenced by CONMINOptimizer::allocate_workspace(), and CONMINOptimizer::core_run().

14.31.3.7 int N4 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N4 = Maximum(N3,number of variables)

Referenced by CONMINOptimizer::allocate_workspace(), and CONMINOptimizer::core_run().

14.31.3.8 int N5 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N5 = 2$*$(N4)

Referenced by CONMINOptimizer::allocate_workspace(), and CONMINOptimizer::core_run().

14.31.3.9 double CT [private]

Constraint thickness parameter.

The value of CT decreases in magnitude during optimization.

Referenced by CONMINOptimizer::core_run(), and CONMINOptimizer::initialize().

14.31.3.10 double* S [private]

Internal CONMIN array.

Move direction in N-dimensional space.

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

14.31.3.11 double* G1 [private]

Internal CONMIN array.

Temporary storage of constraint values.

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

14.31.3.12 double* G2 [private]

Internal CONMIN array.

Temporary storage of constraint values.

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

14.31.3.13 double* B [private]

Internal CONMIN array.

Temporary storage for computations involving array S.

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

14.31.3.14 double* C [private]

Internal CONMIN array.

Temporary storage for use with arrays B and S.

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

14.31.3.15 int* MS1 [private]

Internal CONMIN array.

Temporary storage for use with arrays B and S.

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

14.31.3.16 double* SCAL [private]

Internal CONMIN array.

Vector of scaling parameters for design parameter values.

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

14.31.3.17 double* DF [private]

Internal CONMIN array.

Temporary storage for analytic gradient data.

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

14.31.3.18 double* A [private]

Internal CONMIN array.

Temporary 2-D array for storage of constraint gradients.

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), and CONMINOptimizer::deallocate_workspace().

14.31.3.19 int* ISC [private]

Internal CONMIN array.

Array of flags to identify linear constraints. (not used in this implementation of CONMIN)

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), CONMINOptimizer::deallocate_workspace(), and CONMINOptimizer::initialize_run().

14.31.3.20 int* IC [private]

Internal CONMIN array.

Array of flags to identify active and violated constraints

Referenced by CONMINOptimizer::allocate_workspace(), CONMINOptimizer::core_run(), CONMINOptimizer::deallocate_workspace(), and CONMINOptimizer::initialize_run().

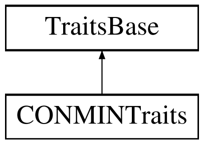
The documentation for this class was generated from the following files:

- CONMINOptimizer.hpp
- CONMINOptimizer.cpp

14.32 CONMINTraits Class Reference

A version of TraitsBase specialized for CONMIN optimizers.

Inheritance diagram for CONMINTraits:



Public Member Functions

- CONMINTraits ()
  default constructor
- virtual ∼CONMINTraits ()
  destructor
- virtual bool is_derived ()
  A temporary query used in the refactor.
- bool supports_continuous_variables ()
  Return the flag indicating whether method supports continuous variables.
- bool supports_linear_equality ()
  Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()
  Return the flag indicating whether method supports linear inequalities.
- LINEAR_INEQUALITY_FORMAT linear_inequality_format ()
  Return the format used for linear inequality constraints.
- bool supports_nonlinear_equality ()
  Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()
  Return the flag indicating whether method supports nonlinear inequalities.
- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()
  Return the format used for nonlinear inequality constraints.

14.32.1 Detailed Description

A version of TraitsBase specialized for CONMIN optimizers.

The documentation for this class was generated from the following file:

- CONMINOptimizer.hpp

14.33 ConsoleRedirector Class Reference

Public Member Functions

- ConsoleRedirector (std::ostream ∗&dakota_stream, std::ostream ∗default_dest)
  Constructor taking a reference to the Dakota Cout/Cerr handle and a default destination to use when no redirection (or destruct)
- ∼ConsoleRedirector ()
  when the redirector stack is destroyed, it will rebind the output handle to the default ostream, then destroy open files
- void push_back ()
  push back the default or repeat the last pushed file stream
- void push_back (const String &filename)
  push back a new output filestream, or repeat the last one if no filename change
- void pop_back ()
  pop the last redirection

Protected Attributes

- std::ostream ∗& ostreamHandle

  The handle (target ostream) through which output is sent; typically dakota_cout or dakota_cerr. Will be rebound to specific streams as they are pushed or popped.
- std::ostream ∗ defaultOStream

  initial stream to reset to when redirections are done (typically std::cout or std::cerr)
- std::vector< std::shared_ptr
  < OutputWriter > > ostreamDestinations

  stack of redirections to OutputWriters; shared pointers are used to potentially share the same ostream at multiple levels

Private Member Functions

- ConsoleRedirector ()

  default constructor is disallowed
- ConsoleRedirector (const ConsoleRedirector &)

  copy constructor is disallowed due
- const ConsoleRedirector & operator= (const ConsoleRedirector &)

  assignment is disallowed

14.33.1 Detailed Description

Component to manage a set of output or error redirections. Push operations may present a new filename, or none in order to preserve current binding to cout/cerr or file, but place an entry on the stack. Cout/Cerr are rebound as needed when a stream is destroyed on pop.

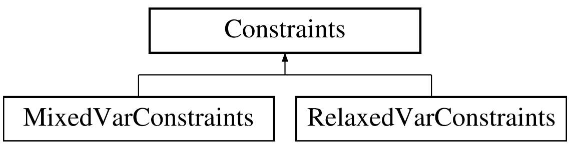
The documentation for this class was generated from the following files:

- OutputManager.hpp
- OutputManager.cpp

14.34 Constraints Class Reference

Base class for the variable constraints class hierarchy.

Inheritance diagram for Constraints:



Public Member Functions

- Constraints ()

  default constructor
- Constraints (const ProblemDescDB &prob_db, const SharedVariablesData &svd)

  standard constructor
- Constraints (const SharedVariablesData &svd)

  alternate constructor for instantiations on the fly

- Constraints (const Constraints &con)

  copy constructor
- virtual ∼Constraints ()

  destructor
- Constraints operator= (const Constraints &con)

  assignment operator
- virtual void write (std::ostream &s) const

  write a variable constraints object to an std::ostream
- virtual void read (std::istream &s)

  read a variable constraints object from an std::istream
- const RealVector & continuous_lower_bounds () const

  return the active continuous variable lower bounds
- Real continuous_lower_bound (size_t i) const

  return an active continuous variable lower bound
- void continuous_lower_bounds (const RealVector &cl_bnds)

  set the active continuous variable lower bounds
- void continuous_lower_bound (Real cl_bnd, size_t i)

  set an active continuous variable lower bound
- const RealVector & continuous_upper_bounds () const

  return the active continuous variable upper bounds
- Real continuous_upper_bound (size_t i) const

  return an active continuous variable upper bound
- void continuous_upper_bounds (const RealVector &cu_bnds)

  set the active continuous variable upper bounds
- void continuous_upper_bound (Real cu_bnd, size_t i)

  set an active continuous variable upper bound
- const IntVector & discrete_int_lower_bounds () const

  return the active discrete variable lower bounds
- int discrete_int_lower_bound (size_t i) const

  return an active discrete variable lower bound
- void discrete_int_lower_bounds (const IntVector &dil_bnds)

  set the active discrete variable lower bounds
- void discrete_int_lower_bound (int dil_bnd, size_t i)

  set an active discrete variable lower bound
- const IntVector & discrete_int_upper_bounds () const

  return the active discrete variable upper bounds
- int discrete_int_upper_bound (size_t i) const

  return an active discrete variable upper bound
- void discrete_int_upper_bounds (const IntVector &diu_bnds)

  set the active discrete variable upper bounds
- void discrete_int_upper_bound (int diu_bnd, size_t i)

  set an active discrete variable upper bound
- const RealVector & discrete_real_lower_bounds () const

  return the active discrete variable lower bounds
- Real discrete_real_lower_bound (size_t i) const

  return an active discrete variable lower bound
- void discrete_real_lower_bounds (const RealVector &drl_bnds)

  set the active discrete variable lower bounds
- void discrete_real_lower_bound (Real drl_bnd, size_t i)

  set an active discrete variable lower bound
- const RealVector & discrete_real_upper_bounds () const

return the active discrete variable upper bounds
- Real discrete_real_upper_bound (size_t i) const

  return an active discrete variable upper bound
- void discrete_real_upper_bounds (const RealVector &dru_bnds)

  set the active discrete variable upper bounds
- void discrete_real_upper_bound (Real dru_bnd, size_t i)

  set an active discrete variable upper bound
- const RealVector & inactive_continuous_lower_bounds () const

  return the inactive continuous lower bounds
- void inactive_continuous_lower_bounds (const RealVector &icl_bnds)

  set the inactive continuous lower bounds
- const RealVector & inactive_continuous_upper_bounds () const

  return the inactive continuous upper bounds
- void inactive_continuous_upper_bounds (const RealVector &icu_bnds)

  set the inactive continuous upper bounds
- const IntVector & inactive_discrete_int_lower_bounds () const

  return the inactive discrete lower bounds
- void inactive_discrete_int_lower_bounds (const IntVector &idil_bnds)

  set the inactive discrete lower bounds
- const IntVector & inactive_discrete_int_upper_bounds () const

  return the inactive discrete upper bounds
- void inactive_discrete_int_upper_bounds (const IntVector &idiu_bnds)

  set the inactive discrete upper bounds
- const RealVector & inactive_discrete_real_lower_bounds () const

  return the inactive discrete lower bounds
- void inactive_discrete_real_lower_bounds (const RealVector &idrl_bnds)

  set the inactive discrete lower bounds
- const RealVector & inactive_discrete_real_upper_bounds () const

  return the inactive discrete upper bounds
- void inactive_discrete_real_upper_bounds (const RealVector &idru_bnds)

  set the inactive discrete upper bounds
- const RealVector & all_continuous_lower_bounds () const

  returns a single array with all continuous lower bounds
- void all_continuous_lower_bounds (const RealVector &acl_bnds)

  sets all continuous lower bounds using a single array
- void all_continuous_lower_bound (Real acl_bnd, size_t i)

  set a lower bound within the all continuous lower bounds array
- const RealVector & all_continuous_upper_bounds () const

  returns a single array with all continuous upper bounds
- void all_continuous_upper_bounds (const RealVector &acu_bnds)

  sets all continuous upper bounds using a single array
- void all_continuous_upper_bound (Real acu_bnd, size_t i)

  set an upper bound within the all continuous upper bounds array
- const IntVector & all_discrete_int_lower_bounds () const

  returns a single array with all discrete lower bounds
- void all_discrete_int_lower_bounds (const IntVector &adil_bnds)

  sets all discrete lower bounds using a single array
- void all_discrete_int_lower_bound (int adil_bnd, size_t i)

  set a lower bound within the all discrete lower bounds array
- const IntVector & all_discrete_int_upper_bounds () const

  returns a single array with all discrete upper bounds

- void all_discrete_int_upper_bounds (const IntVector &adiu_bnds)

  sets all discrete upper bounds using a single array
- void all_discrete_int_upper_bound (int adiu_bnd, size_t i)

  set an upper bound within the all discrete upper bounds array
- const RealVector & all_discrete_real_lower_bounds () const

  returns a single array with all discrete lower bounds
- void all_discrete_real_lower_bounds (const RealVector &adrl_bnds)

  sets all discrete lower bounds using a single array
- void all_discrete_real_lower_bound (Real adrl_bnd, size_t i)

  set a lower bound within the all discrete lower bounds array
- const RealVector & all_discrete_real_upper_bounds () const

  returns a single array with all discrete upper bounds
- void all_discrete_real_upper_bounds (const RealVector &adru_bnds)

  sets all discrete upper bounds using a single array
- void all_discrete_real_upper_bound (Real adru_bnd, size_t i)

  set an upper bound within the all discrete upper bounds array
- size_t num_linear_ineq_constraints () const

  return the number of linear inequality constraints
- size_t num_linear_eq_constraints () const

  return the number of linear equality constraints
- const RealMatrix & linear_ineq_constraint_coeffs () const

  return the linear inequality constraint coefficients
- void linear_ineq_constraint_coeffs (const RealMatrix &lin_ineq_coeffs)

  set the linear inequality constraint coefficients
- const RealVector & linear_ineq_constraint_lower_bounds () const

  return the linear inequality constraint lower bounds
- void linear_ineq_constraint_lower_bounds (const RealVector &lin_ineq_l_bnds)

  set the linear inequality constraint lower bounds
- const RealVector & linear_ineq_constraint_upper_bounds () const

  return the linear inequality constraint upper bounds
- void linear_ineq_constraint_upper_bounds (const RealVector &lin_ineq_u_bnds)

  set the linear inequality constraint upper bounds
- const RealMatrix & linear_eq_constraint_coeffs () const

  return the linear equality constraint coefficients
- void linear_eq_constraint_coeffs (const RealMatrix &lin_eq_coeffs)

  set the linear equality constraint coefficients
- const RealVector & linear_eq_constraint_targets () const

  return the linear equality constraint targets
- void linear_eq_constraint_targets (const RealVector &lin_eq_targets)

  set the linear equality constraint targets
- size_t num_nonlinear_ineq_constraints () const

  return the number of nonlinear inequality constraints
- size_t num_nonlinear_eq_constraints () const

  return the number of nonlinear equality constraints
- const RealVector & nonlinear_ineq_constraint_lower_bounds () const

  return the nonlinear inequality constraint lower bounds
- void nonlinear_ineq_constraint_lower_bounds (const RealVector &nln_ineq_l_bnds)

  set the nonlinear inequality constraint lower bounds
- const RealVector & nonlinear_ineq_constraint_upper_bounds () const

  return the nonlinear inequality constraint upper bounds
- void nonlinear_ineq_constraint_upper_bounds (const RealVector &nln_ineq_u_bnds)

set the nonlinear inequality constraint upper bounds

- const RealVector & nonlinear_eq_constraint_targets () const

  return the nonlinear equality constraint targets

- void nonlinear_eq_constraint_targets (const RealVector &nln_eq_targets)

  set the nonlinear equality constraint targets

- Constraints copy () const

  for use when a deep copy is needed (the representation is not shared)

- void update (const Constraints &cons)

  for use when only data updates are desired between existing Constraints objects

- void shape ()

  shape the lower/upper bound arrays based on sharedVarsData

- void reshape (size_t num_nln_ineq_cons, size_t num_nln_eq_cons, size_t num_lin_ineq_cons, size_t num_lin_eq_cons, const SharedVariablesData &svd)

  reshape the linear/nonlinear/bound constraint arrays arrays and the lower/upper bound arrays

- void reshape ()

  reshape the lower/upper bound arrays based on sharedVarsData

- void reshape (size_t num_nln_ineq_cons, size_t num_nln_eq_cons, size_t num_lin_ineq_cons, size_t num_lin_eq_cons)

  reshape the linear/nonlinear constraint arrays

- void inactive_view (short view2)

  sets the inactive view based on higher level (nested) context

- bool is_null () const

  function to check constraintsRep (does this envelope contain a letter)

Protected Member Functions

- Constraints (BaseConstructor, const ProblemDescDB &problem_db, const SharedVariablesData &svd)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

- Constraints (BaseConstructor, const SharedVariablesData &svd)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

- void build_views ()

  construct active/inactive views of all variables arrays

- void build_active_views ()

  construct active views of all variables bounds arrays

- void build_inactive_views ()

  construct inactive views of all variables bounds arrays

- void manage_linear_constraints (const ProblemDescDB &problem_db)

  perform checks on user input, convert linear constraint coefficient input to matrices, and assign defaults

Protected Attributes

- SharedVariablesData sharedVarsData

  configuration data shared from a Variables instance

- RealVector allContinuousLowerBnds

  a continuous lower bounds array combining continuous design, uncertain, and continuous state variable types (all view).

- RealVector allContinuousUpperBnds

  a continuous upper bounds array combining continuous design, uncertain, and continuous state variable types (all view).

- IntVector allDiscreteIntLowerBnds

  a discrete lower bounds array combining discrete design and discrete state variable types (all view).
- IntVector allDiscreteIntUpperBnds

  a discrete upper bounds array combining discrete design and discrete state variable types (all view).
- RealVector allDiscreteRealLowerBnds

  a discrete lower bounds array combining discrete design and discrete state variable types (all view).
- RealVector allDiscreteRealUpperBnds

  a discrete upper bounds array combining discrete design and discrete state variable types (all view).
- size_t numNonlinearIneqCons

  number of nonlinear inequality constraints
- size_t numNonlinearEqCons

  number of nonlinear equality constraints
- RealVector nonlinearIneqConLowerBnds

  nonlinear inequality constraint lower bounds
- RealVector nonlinearIneqConUpperBnds

  nonlinear inequality constraint upper bounds
- RealVector nonlinearEqConTargets

  nonlinear equality constraint targets
- size_t numLinearIneqCons

  number of linear inequality constraints
- size_t numLinearEqCons

  number of linear equality constraints
- RealMatrix linearIneqConCoeffs

  linear inequality constraint coefficients
- RealMatrix linearEqConCoeffs

  linear equality constraint coefficients
- RealVector linearIneqConLowerBnds

  linear inequality constraint lower bounds
- RealVector linearIneqConUpperBnds

  linear inequality constraint upper bounds
- RealVector linearEqConTargets

  linear equality constraint targets
- RealVector continuousLowerBnds

  the active continuous lower bounds array view
- RealVector continuousUpperBnds

  the active continuous upper bounds array view
- IntVector discreteIntLowerBnds

  the active discrete lower bounds array view
- IntVector discreteIntUpperBnds

  the active discrete upper bounds array view
- RealVector discreteRealLowerBnds

  the active discrete lower bounds array view
- RealVector discreteRealUpperBnds

  the active discrete upper bounds array view
- RealVector inactiveContinuousLowerBnds

  the inactive continuous lower bounds array view
- RealVector inactiveContinuousUpperBnds

  the inactive continuous upper bounds array view
- IntVector inactiveDiscreteIntLowerBnds

  the inactive discrete lower bounds array view
- IntVector inactiveDiscreteIntUpperBnds

the inactive discrete upper bounds array view

- RealVector inactiveDiscreteRealLowerBnds

  the inactive discrete lower bounds array view
- RealVector inactiveDiscreteRealUpperBnds

  the inactive discrete upper bounds array view

Private Member Functions

- std::shared_ptr< Constraints > get_constraints (const ProblemDescDB &problem_db, const SharedVariablesData &svd)

  Used only by the constructor to initialize constraintsRep to the appropriate derived type.
- std::shared_ptr< Constraints > get_constraints (const SharedVariablesData &svd) const

  Used by copy() to initialize constraintsRep to the appropriate derived type.

Private Attributes

- std::shared_ptr< Constraints > constraintsRep

  pointer to the letter (initialized only for the envelope)

14.34.1 Detailed Description

Base class for the variable constraints class hierarchy.

The Constraints class is the base class for the class hierarchy managing bound, linear, and nonlinear constraints. Using the variable lower and upper bounds arrays from the input specification, different derived classes define different views of this data. The linear and nonlinear constraint data is consistent in all views and is managed at the base class level. For memory efficiency and enhanced polymorphism, the variable constraints hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Constraints) serves as the envelope and one of the derived classes (selected in Constraints::get_constraints()) serves as the letter.

14.34.2 Constructor & Destructor Documentation

14.34.2.1 Constraints ( )

default constructor

The default constructor: constraintsRep is NULL in this case (a populated problem_db is needed to build a meaningful Constraints object).

14.34.2.2 Constraints (const ProblemDescDB & *problem_db*, const SharedVariablesData & *svd*)

standard constructor

The envelope constructor only needs to extract enough data to properly execute get_constraints, since the constructor overloaded with BaseConstructor builds the actual base class data inherited by the derived classes.

References Dakota::abort_handler(), and Constraints::constraintsRep.

14.34.2.3 Constraints (const SharedVariablesData & *svd*)

alternate constructor for instantiations on the fly

Envelope constructor for instantiations on the fly. This constructor executes get_constraints(view), which invokes the default derived/base constructors, followed by a reshape() based on vars_comps.

References Dakota::abort_handler(), and Constraints::constraintsRep.

14.34.2.4 Constraints (const Constraints & *con*)

copy constructor

Copy constructor manages sharing of constraintsRep

References Constraints::constraintsRep.

14.34.2.5 Constraints (BaseConstructor , const ProblemDescDB & *problem_db*, const SharedVariablesData & *svd*) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_constraints() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_constraints() again). Since the letter IS the representation, its rep pointer is set to NULL.

References Constraints::build_views(), Constraints::manage_linear_constraints(), and Constraints::shape().

14.34.2.6 Constraints (BaseConstructor , const SharedVariablesData & *svd*) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_constraints() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_constraints() again). Since the letter IS the representation, its rep pointer is set to NULL.

References Constraints::build_views(), and Constraints::shape().

14.34.3 Member Function Documentation

14.34.3.1 Constraints operator= (const Constraints & *con*)

assignment operator

Assignment operator shares the constraintsRep with this envelope.

References Constraints::constraintsRep.

14.34.3.2 Constraints copy ( ) const

for use when a deep copy is needed (the representation is *not* shared)

Deep copies are used for history mechanisms that catalogue permanent copies (should not change as the representation within userDefinedConstraints changes).

References Constraints::constraintsRep, Constraints::get_constraints(), and Constraints::update().

Referenced by SurrogateModel::force_rebuild(), and RecastModel::init_constraints().

14.34.3.3 void update (const Constraints & *cons*)

for use when only data updates are desired between existing Constraints objects

Deep copies are used for history mechanisms that catalogue permanent copies (should not change as the representation within userDefinedConstraints changes).

References Constraints::constraintsRep.

Referenced by AdapterModel::AdapterModel(), and Constraints::copy().

14.34.3.4 void shape ( )

shape the lower/upper bound arrays based on sharedVarsData

Resizes the derived bounds arrays.

References SharedVariablesData::all_counts(), Constraints::allContinuousLowerBnds, Constraints::allContinuousUpperBnds, Constraints::allDiscreteIntLowerBnds, Constraints::allDiscreteIntUpperBnds, Constraints::allDiscreteRealLowerBnds, Constraints::allDiscreteRealUpperBnds, Constraints::constraintsRep, and Constraints::sharedVarsData.

Referenced by Constraints::Constraints().

14.34.3.5 void reshape (size_t *num_nln_ineq_cons,* size_t *num_nln_eq_cons,* size_t *num_lin_ineq_cons,* size_t *num_lin_eq_cons*)

reshape the linear/nonlinear constraint arrays

Resizes the linear and nonlinear constraint arrays at the base class. Does NOT currently resize the derived bounds arrays.

References Constraints::constraintsRep, Constraints::continuousLowerBnds, Constraints::discreteIntLowerBnds, Constraints::discreteRealLowerBnds, Constraints::linearEqConCoeffs, Constraints::linearEqConTargets, Constraints::linearIneqConCoeffs, Constraints::linearIneqConLowerBnds, Constraints::linearIneqConUpperBnds, Constraints::nonlinearEqConTargets, Constraints::nonlinearIneqConLowerBnds, Constraints::nonlinearIneqConUpperBnds, Constraints::numLinearEqCons, Constraints::numLinearIneqCons, Constraints::numNonlinearEqCons, and Constraints::numNonlinearIneqCons.

14.34.3.6 void manage_linear_constraints (const **ProblemDescDB** & *problem_db*) [protected]

perform checks on user input, convert linear constraint coefficient input to matrices, and assign defaults

Convenience function called from derived class constructors. The number of variables active for applying linear constraints is currently defined to be the number of active continuous variables plus the number of active discrete variables (the most general case), even though very few optimizers can currently support mixed variable linear constraints.

References Dakota::abort_handler(), Constraints::continuousLowerBnds, Dakota::copy_data(), Constraints::discreteIntLowerBnds, Constraints::discreteRealLowerBnds, ProblemDescDB::get_rv(), Constraints::linearEqConCoeffs, Constraints::linearEqConTargets, Constraints::linearIneqConCoeffs, Constraints::linearIneqConLowerBnds, Constraints::linearIneqConUpperBnds, Constraints::numLinearEqCons, and Constraints::numLinearIneqCons.

Referenced by Constraints::Constraints().

14.34.3.7 std::shared_ptr< **Constraints** > get_constraints (const **ProblemDescDB** & *problem_db,* const **SharedVariablesData** & *svd*) [private]

Used only by the constructor to initialize constraintsRep to the appropriate derived type.

Initializes constraintsRep to the appropriate derived type, as given by the variables view.

References Dakota::svd(), and SharedVariablesData::view().

Referenced by Constraints::copy().

14.34.3.8 std::shared_ptr< Constraints > get_constraints (const SharedVariablesData & *svd*) const [private]

Used by copy() to initialize constraintsRep to the appropriate derived type.

Initializes constraintsRep to the appropriate derived type, as given by the variables view. The default derived class constructors are invoked.

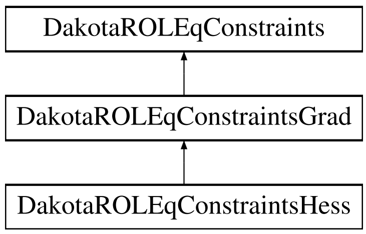
References Dakota::svd(), and SharedVariablesData::view().

The documentation for this class was generated from the following files:

- DakotaConstraints.hpp
- DakotaConstraints.cpp

14.35 DakotaROLEqConstraints Class Reference

Inheritance diagram for DakotaROLEqConstraints:



Public Member Functions

- DakotaROLEqConstraints (Model &model)

  Constructor.
- void value (std::vector< Real > &c, const std::vector< Real > &x, Real &tol) override

  Function to return the constaint value to ROL.

Protected Attributes

- Model & dakotaModel

  Dakota problem data provided by user.
- bool haveNlnConst

  Whether or not problem has nonlinear equality constraints.

14.35.1 Detailed Description

DakotaROLEqConstraints is derived from the ROL constraint class. It overrides the member functions to provide Dakota-specific implementations of equality constraint evaluation and the application of the equality constraint Jacobian to a vector.

14.35.2 Constructor & Destructor Documentation

14.35.2.1 DakotaROLEqConstraints (Model & *model*)

Constructor.

Implementation of the DakotaROLEqConstraints class.

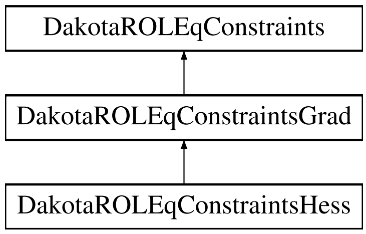
References DakotaROLEqConstraints::haveNlnConst, and Model::num_nonlinear_eq_constraints().

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.36 DakotaROLEqConstraintsGrad Class Reference

Inheritance diagram for DakotaROLEqConstraintsGrad:



Public Member Functions

- DakotaROLEqConstraintsGrad (Model &model)

  Constructor.
- virtual ∼DakotaROLEqConstraintsGrad ()

  Destructor.
- void applyJacobian (std::vector< Real > &jv, const std::vector< Real > &v, const std::vector< Real > &x, Real &tol) override

  Function to return the result of applying the constraint gradient to an arbitrary vector to ROL.
- void applyAdjointJacobian (std::vector< Real > &ajv, const std::vector< Real > &v, const std::vector< Real > &x, Real &tol) override

  Function to return the result of applying the constraint adjoint to an arbitrary vector to ROL.

Additional Inherited Members

14.36.1 Detailed Description

DakotaROLEqConstraintsGrad is derived from DakotaROLEqConstraints. It implements overrides of ROL member functions to provide a Dakota-specific application of the inequality constraint Jacobian to a vector. This separate class is needed to allow for the option of utilizing ROL's finite-differenced gradients

14.36.2 Constructor & Destructor Documentation

14.36.2.1 DakotaROLEqConstraintsGrad (Model & *model*)

Constructor.

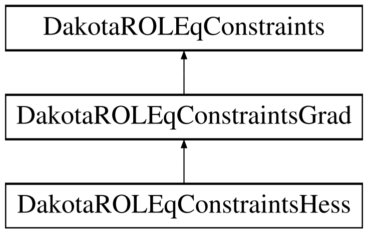
Implementation of the DakotaROLEqConstraintsGrad class.

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.37 DakotaROLEqConstraintsHess Class Reference

Inheritance diagram for DakotaROLEqConstraintsHess:



Public Member Functions

- DakotaROLEqConstraintsHess (Model &model)

    Constructor.
- virtual ∼DakotaROLEqConstraintsHess ()

    Destructor.
- void applyAdjointHessian (std::vector< Real > &ahuv, const std::vector< Real > &u, const std::vector< Real > &v, const std::vector< Real > &x, Real &tol) override

    Function to return the result of applying the constraint adjoint Hessian to an arbitrary vector to ROL.

Additional Inherited Members

14.37.1 Detailed Description

DakotaROLEqConstraintsHess is derived from DakotaROLEqConstraintsGrad. It implements overrides of ROL member functions to provide a Dakota-specific implementation of a adjoint Hessian-vector product for equality constraints. This separate class is needed (rather than putting the product into DakotaROLEqConstraints) because logic in ROL does not always protect against calling the adjoint Hessian-vector product in cases where there is not actually a Hessian provided.

14.37.2 Constructor & Destructor Documentation

14.37.2.1 DakotaROLEqConstraintsHess (Model & *model*)

Constructor.

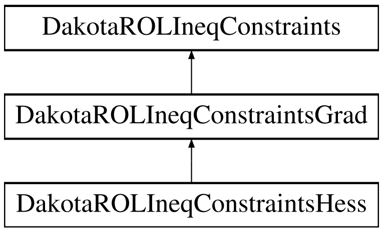
Implementation of the DakotaROLEqConstraintsHess class.

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.38 DakotaROLIneqConstraints Class Reference

Inheritance diagram for DakotaROLIneqConstraints:



Public Member Functions

- DakotaROLIneqConstraints (Model &model)

  Constructor.
- void value (std::vector< Real > &c, const std::vector< Real > &x, Real &tol) override

  Function to return the constraint value to ROL.

Protected Attributes

- Model & dakotaModel

  Dakota problem data provided by user.
- bool haveNlnConst

  Whether or not problem has nonlinear inequality constraints.

14.38.1 Detailed Description

DakotaROLIneqConstraints is derived from the ROL constraint class. It overrides the member functions to provide Dakota-specific implementations of inequality constraint evaluation.

14.38.2 Constructor & Destructor Documentation

14.38.2.1 DakotaROLIneqConstraints (Model & *model*)

Constructor.

Implementation of the DakotaROLIneqConstraints class.

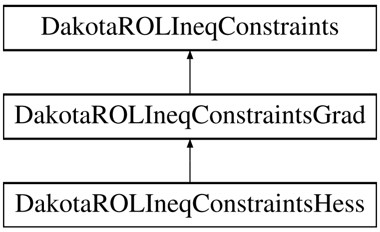
References DakotaROLIneqConstraints::haveNlnConst, and Model::num_nonlinear_ineq_constraints().

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.39 DakotaROLIneqConstraintsGrad Class Reference

Inheritance diagram for DakotaROLIneqConstraintsGrad:



Public Member Functions

- DakotaROLIneqConstraintsGrad (Model &model)

    Constructor.

- virtual ∼DakotaROLIneqConstraintsGrad ()

    Destructor.

- void applyJacobian (std::vector< Real > &jv, const std::vector< Real > &v, const std::vector< Real > &x, Real &tol) override

    Function to return the result of applying the constraint gradient on an arbitrary vector to ROL.

- void applyAdjointJacobian (std::vector< Real > &ajv, const std::vector< Real > &v, const std::vector< Real > &x, Real &tol) override

    Function to return the result of applying the constraint adjoint to an arbitrary vector to ROL.

Additional Inherited Members

14.39.1 Detailed Description

DakotaROLIneqConstraintsGrad is derived from DakotaROLIneqConstraints. It implements overrides of ROL member functions to provide a Dakota-specific application of the inequality constraint Jacobian to a vector. This separate class is needed to allow for the option of utilizing ROL's finite-differenced gradients

14.39.2 Constructor & Destructor Documentation

14.39.2.1 DakotaROLIneqConstraintsGrad (Model & *model*)

Constructor.

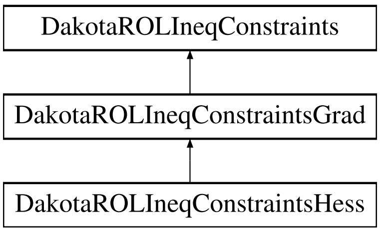
Implementation of the DakotaROLIneqConstraintsGrad class.

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.40 DakotaROLIneqConstraintsHess Class Reference

Inheritance diagram for DakotaROLIneqConstraintsHess:



Public Member Functions

- DakotaROLIneqConstraintsHess (Model &model)

    Constructor.
- virtual ∼DakotaROLIneqConstraintsHess ()

    Destructor.
- void applyAdjointHessian (std::vector< Real > &ahuv, const std::vector< Real > &u, const std::vector< Real > &v, const std::vector< Real > &x, Real &tol) override

    Function to return the result of applying the constraint adjoint Hessian to an arbitrary vector to ROL.

Additional Inherited Members

14.40.1 Detailed Description

DakotaROLIneqConstraintsHess is derived from DakotaROLIneqConstraintsGrad. It implements overrides of ROL member functions to provide a Dakota-specific implementation of a adjoint Hessian-vector product for inequality constraints. This separate class is needed (rather than putting the product into DakotaROLIneqConstraints) because logic in ROL does not always protect against calling the adjoint Hessian-vector product in cases where there is not actually a Hessian provided.

14.40.2 Constructor & Destructor Documentation

14.40.2.1 DakotaROLIneqConstraintsHess (Model & *model*)

Constructor.

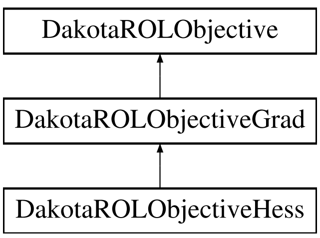
Implementation of the DakotaROLIneqConstraintsGrad class.

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.41 DakotaROLObjective Class Reference

Inheritance diagram for DakotaROLObjective:



Public Member Functions

- DakotaROLObjective (Model &model)

  Constructor.
- Real value (const std::vector< Real > &x, Real &tol) override

  Function to return the objective value (response) to ROL.

Public Attributes

- Model & dakotaModel

  Dakota problem data provided by user.

14.41.1 Detailed Description

DakotaROLObjective is derived from the ROL objective class. It overrides the member functions to provide Dakota-specific implementations of function evaluations.

14.41.2 Constructor & Destructor Documentation

14.41.2.1 DakotaROLObjective (Model & *model*)

Constructor.

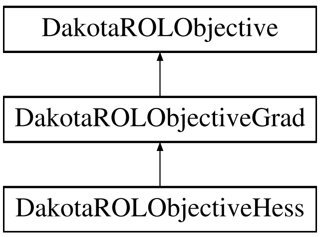
Implementation of the DakotaROLObjective class.

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.42 DakotaROLObjectiveGrad Class Reference

Inheritance diagram for DakotaROLObjectiveGrad:



Public Member Functions

- DakotaROLObjectiveGrad (Model &model)

  Constructor.
- virtual ~DakotaROLObjectiveGrad ()

  Destructor.
- void gradient (std::vector< Real > &g, const std::vector< Real > &x, Real &tol) override

  Function to return the response gradient to ROL.

Additional Inherited Members

14.42.1 Detailed Description

DakotaROLObjectiveGrad is derived from DakotaROLObjective. It implements overrides of ROL member functions to provide a Dakota-specific Gradient support for the objective function. This separate class is needed to allow for the option of utilizing ROL's finite-differenced gradients

14.42.2 Constructor & Destructor Documentation

14.42.2.1 DakotaROLObjectiveGrad (Model & *model*)

Constructor.

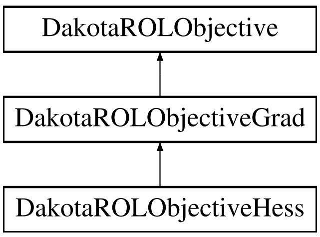
Implementation of the DakotaROLObjectiveGrad class.

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.43 DakotaROLObjectiveHess Class Reference

Inheritance diagram for DakotaROLObjectiveHess:



Public Member Functions

- DakotaROLObjectiveHess (Model &model)
  Constructor.
- virtual ~DakotaROLObjectiveHess ()
  Destructor.
- void hessVec (std::vector< Real > &hv, const std::vector< Real > &v, const std::vector< Real > &x, Real &tol) override
  Function to return Hessian-vector product needed by ROL when using user/Dakota-supplied Hessians.
- void invHessVec (std::vector< Real > &hv, const std::vector< Real > &v, const std::vector< Real > &x, Real &tol) override
  This function is not used by ROL algorithms currently supported by Dakota but is included to protect against unexpected behavior.

Additional Inherited Members

14.43.1 Detailed Description

DakotaROLObjectiveHess is derived from DakotaROLObjectiveGrad. It implements overrides of ROL member functions to provide a Dakota-specific implementation of a Hessian-vector product. This separate class is needed (rather than putting the product into DakotaROLObjective) because logic in ROL does not always protect against calling the Hessian-vector product in cases where there is not actually a Hessian provided.

14.43.2 Constructor & Destructor Documentation

14.43.2.1 DakotaROLObjectiveHess (Model & *model*)

Constructor.

Implementation of the DakotaROLObjectiveHess class.

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.44 DataEnvironment Class Reference

Handle class for environment specification data.

Public Member Functions

- DataEnvironment ()

  constructor
- DataEnvironment (const DataEnvironment &)

  copy constructor
- ∼DataEnvironment ()

  destructor
- DataEnvironment & operator= (const DataEnvironment &)

  assignment operator
- void write (std::ostream &s) const

  write a DataEnvironment object to an std::ostream
- void read (MPIUnpackBuffer &s)

  read a DataEnvironment object from a packed MPI buffer
- void write (MPIPackBuffer &s) const

  write a DataEnvironment object to a packed MPI buffer
- std::shared_ptr
  < DataEnvironmentRep > data_rep ()

  return dataEnvRep

Private Attributes

- std::shared_ptr
  < DataEnvironmentRep > dataEnvRep

  pointer to the body (handle-body idiom)

Friends

- class **ProblemDescDB**
- class **NIDRProblemDescDB**

14.44.1 Detailed Description

Handle class for environment specification data.

The DataEnvironment class is used to provide a memory management handle for the data in DataEnvironmentRep. It is populated by IDRProblemDescDB::environment_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A single DataEnvironment object is maintained in ProblemDescDB::environmentSpec.

The documentation for this class was generated from the following files:

- DataEnvironment.hpp
- DataEnvironment.cpp

14.45 DataEnvironmentRep Class Reference

Body class for environment specification data.

Public Member Functions

- ∼DataEnvironmentRep ()

  destructor (public for shared_ptr)

Public Attributes

- bool checkFlag

  flag for whether to run in check only mode (default false)
- String outputFile

  file name for output redirection (overrides command-line)
- String errorFile

  file name for error redirection (overrides command-line)
- String readRestart

  file name for restart read (overrides command-line)
- int stopRestart

  record at which to stop reading restart
- String writeRestart

  file name for restart write (overrides command-line)
- bool preRunFlag

  flags invocation with command line option -pre_run
- bool runFlag

  flags invocation with command line option -run
- bool postRunFlag

  flags invocation with command line option -post_run
- String preRunInput

  filename for pre_run input
- String preRunOutput

  filename for pre_run output
- String runInput

  filename for run input
- String runOutput

  filename for run output
- String postRunInput

filename for post_run input

- String postRunOutput

  filename for post_run output

- unsigned short preRunOutputFormat

  tabular format for pre_run output

- unsigned short postRunInputFormat

  tabular format for post_run input

- bool graphicsFlag

  flags use of graphics by the environment (from the `graphics` specification in EnvIndControl)

- bool tabularDataFlag

  flags tabular data collection by the environment (from the tabular_graphics_data specification in EnvIndControl)

- String tabularDataFile

  the filename used for tabular data collection by the environment (from the tabular_graphics_file specification in Env-IndControl)

- unsigned short tabularFormat

  format for tabular data files (see enum)

- int outputPrecision

  output precision for tabular and screen output

- bool resultsOutputFlag

  flags use of results output to default file

- String resultsOutputFile

  named file for results output

- unsigned short resultsOutputFormat

  Results output format.

- unsigned short modelEvalsSelection

  Model selection for eval storage.

- unsigned short interfEvalsSelection

  Interface selection for eval storage.

- String topMethodPointer

  method identifier for the environment (from the `top_method_pointer` specification

Private Member Functions

- DataEnvironmentRep ()

  constructor

- void write (std::ostream &s) const

  write a DataEnvironmentRep object to an std::ostream

- void read (MPIUnpackBuffer &s)

  read a DataEnvironmentRep object from a packed MPI buffer

- void write (MPIPackBuffer &s) const

  write a DataEnvironmentRep object to a packed MPI buffer

Friends

- class DataEnvironment

  the handle class can access attributes of the body class directly

14.45.1 Detailed Description

Body class for environment specification data.

The DataEnvironmentRep class is used to contain the data from the environment keyword specification. Default values are managed in the DataEnvironmentRep constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::environmentSpec is private.

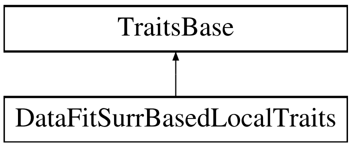
The documentation for this class was generated from the following files:

- DataEnvironment.hpp
- DataEnvironment.cpp

14.46 DataFitSurrBasedLocalTraits Class Reference

Class for provably-convergent local surrogate-based optimization and nonlinear least squares.

Inheritance diagram for DataFitSurrBasedLocalTraits:



Public Member Functions

- DataFitSurrBasedLocalTraits ()

  default constructor
- virtual ~DataFitSurrBasedLocalTraits ()

  destructor
- virtual bool is_derived ()

  A temporary query used in the refactor.
- bool supports_continuous_variables ()

  Return the flag indicating whether method supports continuous variables.
- bool supports_linear_equality ()

  Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()

  Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()

  Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

  Return the flag indicating whether method supports nonlinear inequalities.

14.46.1 Detailed Description

Class for provably-convergent local surrogate-based optimization and nonlinear least squares.

This minimizer uses a SurrogateModel to perform minimization based on local, global, or hierarchical surrogates. It achieves provable convergence through the use of a sequence of trust regions and the application of surrogate corrections at the trust region centers. A version of TraitsBase specialized for local surrogate-based minimizer

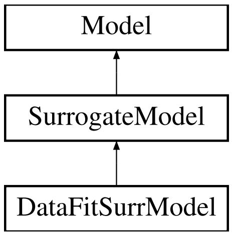
The documentation for this class was generated from the following file:

- DataFitSurrBasedLocalMinimizer.hpp

14.47 DataFitSurrModel Class Reference

Derived model class within the surrogate model branch for managing data fit surrogates (global and local)

Inheritance diagram for DataFitSurrModel:



Public Member Functions

- DataFitSurrModel (ProblemDescDB &problem_db)

    constructor
- DataFitSurrModel (Iterator &dace_iterator, Model &actual_model, const ActiveSet &set, const String &approx-_type, const UShortArray &approx_order, short corr_type, short corr_order, short data_order, short output-_level, const String &point_reuse, const String &import_build_points_file=String(), unsigned short import_-build_format=TABULAR_ANNOTATED, bool import_build_active_only=false, const String &export_approx_-points_file=String(), unsigned short export_approx_format=TABULAR_ANNOTATED)

    alternate constructor for instantiations on the fly
- ∼DataFitSurrModel ()

    destructor
- void total_points (int points)

    set pointsTotal and pointsManagement mode
- int required_points ()

    return points required for build according to pointsManagement mode
- void declare_sources ()

    Declare a model's sources to the evaluationsDB.

Protected Member Functions

- size_t qoi () const

    return number of unique response functions (managing any aggregations)
- DiscrepancyCorrection & discrepancy_correction ()

    return the DiscrepancyCorrection object used by SurrogateModels
- short correction_type ()

    return the correction type from the DiscrepancyCorrection object used by SurrogateModels
- void correction_type (short corr_type)

    set the correction type from the DiscrepancyCorrection object used by SurrogateModels
- short correction_order ()

    return the correction order from the DiscrepancyCorrection object used by SurrogateModels
- bool initialize_mapping (ParLevLIter pl_iter)

    Perform any global updates prior to individual evaluate() calls; returns true if the variables size has changed.
- bool finalize_mapping ()
- void update_model (Model &model)

    update model with data that could change per function evaluation (active variable values/bounds)
- void update_from_model (const Model &model)

update current variables/labels/bounds/targets with data from model

- void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

  set primaryA{C,DI,DS,DR}VarMapIndices, secondaryA{C,DI,DS,DR}VarMapTargets (coming from a higher-level NestedModel context to inform derivative est.)
- const SizetArray & nested_acv1_indices () const

  return primaryACVarMapIndices
- const ShortArray & nested_acv2_targets () const

  return secondaryACVarMapTargets
- short query_distribution_parameter_derivatives () const

  calculate and return derivative composition of final results w.r.t. distribution parameters (none, all, or mixed)
- void check_submodel_compatibility (const Model &sub_model)

  verify compatibility between SurrogateModel attributes and attributes of the submodel (DataFitSurrModel::actualModel or HierarchSurrModel::highFidelityModel)
- void derived_evaluate (const ActiveSet &set)
- void derived_evaluate_nowait (const ActiveSet &set)
- const IntResponseMap & derived_synchronize ()
- const IntResponseMap & derived_synchronize_nowait ()
- void asv_inflate_build (const ShortArray &orig_asv, ShortArray &actual_asv)

  map incoming ASV into actual request for surrogate construction, managing any mismatch in sizes due to response aggregation modes in actualModel
- void asv_split_eval (const ShortArray &orig_asv, ShortArray &actual_asv, ShortArray &approx_asv)

  split incoming ASV into actual and approximate evaluation requests, managing any mismatch in sizes due to response aggregation modes in actualModel
- Iterator & subordinate_iterator ()

  return daceIterator
- void active_model_key (const Pecos::ActiveKey &key)

  set active model key within approxInterface
- void clear_model_keys ()

  remove all model keys within approxInterface
- Model & surrogate_model (size_t i=_NPOS)

  return this model instance
- const Model & surrogate_model (size_t i=_NPOS) const

  return this model instance
- Model & truth_model ()

  return actualModel
- const Model & truth_model () const

  return actualModel
- void derived_subordinate_models (ModelList &ml, bool recurse_flag)

  return actualModel (and optionally its sub-models)
- void resize_from_subordinate_model (size_t depth=SZ_MAX)

  pass request to actualModel if recursing
- void update_from_subordinate_model (size_t depth=SZ_MAX)

  pass request to actualModel if recursing and then update from it
- Interface & derived_interface ()

  return approxInterface
- void primary_response_fn_weights (const RealVector &wts, bool recurse_flag=true)

  set the relative weightings for multiple objective functions or least squares terms and optionally recurses into actualModel
- void surrogate_response_mode (short mode)

  set responseMode and pass any bypass request on to actualModel for any lower-level surrogates.

- void surrogate_function_indices (const SizetSet &surr_fn_indices)

    (re)set the surrogate index set in SurrogateModel::surrogateFnIndices and ApproximationInterface::approxFnIndices
- void build_approximation ()

    Builds the local/multipoint/global approximation using daceIterator/actualModel to generate new data points.
- bool build_approximation (const Variables &vars, const IntResponsePair &response_pr)

    Builds the local/multipoint/global approximation using daceIterator/actualModel to generate new data points that augment the passed vars/response anchor point.
- void rebuild_approximation ()

    Rebuilds the local/multipoint/global approximation using daceIterator/actualModel to generate an increment of appended data.
- void rebuild_approximation (const IntResponsePair &response_pr)

    Rebuilds the local/multipoint/global approximation using the passed response data for a single sample.
- void rebuild_approximation (const IntResponseMap &resp_map)

    Rebuilds the local/multipoint/global approximation using the passed response data for a set of samples.
- void update_approximation (bool rebuild_flag)

    replaces the approximation data with daceIterator results and rebuilds the approximation if requested
- void update_approximation (const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)

    replaces the anchor point, and rebuilds the approximation if requested
- void update_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)

    replaces the current points array and rebuilds the approximation if requested
- void update_approximation (const RealMatrix &samples, const IntResponseMap &resp_map, bool rebuild_-flag)

    replaces the current points array and rebuilds the approximation if requested
- void append_approximation (bool rebuild_flag)

    appends daceIterator results to a global approximation and rebuilds it if requested
- void append_approximation (const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)

    appends a point to a global approximation and rebuilds it if requested
- void append_approximation (const RealMatrix &samples, const IntResponseMap &resp_map, bool rebuild_-flag)

    appends a matrix of points to a global approximation and rebuilds it if requested
- void append_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)

    appends an array of points to a global approximation and rebuilds it if requested
- void append_approximation (const IntVariablesMap &vars_map, const IntResponseMap &resp_map, bool rebuild_flag)

    appends an map of points to a global approximation and rebuilds it if requested
- void replace_approximation (const IntResponsePair &response_pr, bool rebuild_flag)

    replace the response for a single point (based on eval id from response_pr) within an existing surrogate's data
- void replace_approximation (const IntResponseMap &resp_map, bool rebuild_flag)

    replace the responses for a set of points (based on eval ids from resp_map) within an existing surrogate's data
- void track_evaluation_ids (bool track)

    assigns a flag to track evaluation ids within surrogate data, enabling id-based lookups for data replacement
- void pop_approximation (bool save_surr_data, bool rebuild_flag=false)

    remove the previous data set addition to a surrogate (e.g., due to a previous append_approximation() call); flag manages storing of surrogate data for use in a subsequent push_approximation()
- void push_approximation ()

    push a previous approximation data state; reverse of pop_approximation
- bool push_available ()

    query for whether a trial increment is restorable within a surrogate
- void finalize_approximation ()

    finalize an approximation by applying all previous trial increments

- void combine_approximation ()

  combine all level approximations into a separate composite approximation
- void combined_to_active (bool clear_combined=true)

  promote the combined approximation into the active one
- void clear_inactive ()

  clear inactive data stored in the approxInterface
- bool advancement_available ()

  query approxInterface for available advancements in order, rank, etc.
- bool formulation_updated () const

  query approxInterface for updates in formulation (requiring a rebuild)
- void formulation_updated (bool update)

  update the formulation status in approxInterface
- void run_dace ()

  execute the DACE iterator to generate build data
- SharedApproxData & shared_approximation ()

  retrieve the SharedApproxData from approxInterface
- std::vector< Approximation > & approximations ()

  retrieve the set of Approximations from approxInterface
- const RealVectorArray & approximation_coefficients (bool normalized=false)

  return the approximation coefficients from each Approximation (request forwarded to approxInterface)
- void approximation_coefficients (const RealVectorArray &approx_coeffs, bool normalized=false)

  set the approximation coefficients within each Approximation (request forwarded to approxInterface)
- const RealVector & approximation_variances (const Variables &vars)

  return the approximation variance from each Approximation (request forwarded to approxInterface)
- const Pecos::SurrogateData & approximation_data (size_t fn_index)

  return the approximation data from a particular Approximation (request forwarded to approxInterface)
- void component_parallel_mode (short mode)

  update component parallel mode for supporting parallelism in actualModel
- IntIntPair estimate_partition_bounds (int max_eval_concurrency)

  estimate the minimum and maximum partition sizes that can be utilized by this Model
- void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set up actualModel for parallel operations
- void derived_init_serial ()

  set up actualModel for serial operations.
- void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set active parallel configuration within actualModel
- void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  deallocate communicator partitions for the DataFitSurrModel (request forwarded to actualModel)
- void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)

  Service actualModel job requests received from the master. Completes when a termination message is received from stop_servers().
- void stop_servers ()

  Executed by the master to terminate actualModel server operations when DataFitSurrModel iteration is complete.
- void inactive_view (short view, bool recurse_flag=true)

  update the Model's inactive view based on higher level (nested) context and optionally recurse into actualModel
- const String & interface_id () const

  return the approxInterface identifier
- bool evaluation_cache (bool recurse_flag=true) const

  if recurse_flag, return the actualModel evaluation cache usage
- bool restart_file (bool recurse_flag=true) const

  if recurse_flag, return the actualModel restart file usage

- void set_evaluation_reference ()

  set the evaluation counter reference points for the DataFitSurrModel (request forwarded to approxInterface and actual-Model)
- void fine_grained_evaluation_counters ()

  request fine-grained evaluation reporting within approxInterface and actualModel
- void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const

  print the evaluation summary for the DataFitSurrModel (request forwarded to approxInterface and actualModel)
- void warm_start_flag (const bool flag)

  set the warm start flag, including actualModel
- ActiveSet **default_interface_active_set** ()

Protected Attributes

- const bool exportSurrogate

  whether to export the surrogate to file
- const bool autoRefine

  whether to automatically refine the surrogate during the build phase
- const size_t maxIterations

  Maximum number of times to refine the surrogate.
- const size_t maxFuncEvals

  Maximum number of evaluations while refining a surrogate.
- const Real convergenceTolerance

  Convergence criterion, compared to CV score for specified metric.
- const int softConvergenceLimit

  Max number of iterations for which there is no average improvement.
- const String refineCVMetric

  Type of error metric to test for surrogate refinement convegence.
- const int refineCVFolds

  Number of cross validation folds for surrogate refinement.

Private Member Functions

- void import_points (unsigned short tabular_format, bool use_var_labels, bool active_only)

  optionally read surrogate data points from provided file
- void initialize_export ()

  initialize file stream for exporting surrogate evaluations
- void finalize_export ()

  finalize file stream for exporting surrogate evaluations
- void export_point (int eval_id, const Variables &vars, const Response &resp)

  initialize file stream for exporting surrogate evaluations
- void derived_synchronize_approx (bool block, IntResponseMap &approx_resp_map_rekey)

  Common code for processing of approximate response maps shared by derived_synchronize() and derived_-synchronize_nowait()
- void update_local_reference ()

  Updates fit arrays for local or multipoint approximations.
- void build_local_multipoint ()

  Builds a local or multipoint approximation using actualModel.
- void build_local_multipoint (const Variables &vars, const IntResponsePair &response_pr)

  Builds a local or multipoint approximation using actualModel.
- void update_global_reference ()

Updates fit arrays for global approximations.

- void build_global ()

  Builds a global approximation using daceIterator.
- void rebuild_global ()

  Rebuilds a global approximation by generating new data using daceIterator and appending to approxInterface.
- void refine_surrogate ()

  Refine the built surrogate until convergence criteria are met.
- void clear_approx_interface ()

  clear current data from approxInterface
- void update_approx_interface (const Variables &vars, const IntResponsePair &response_pr)

  update anchor data in approxInterface
- void build_approx_interface ()

  build the approxInterface surrogate, passing variable bounds
- bool consistent (const Variables &vars) const

  test if inactive state is consistent
- bool inside (const Variables &vars) const

  test if active vars are within [l_bnds, u_bnds]
- bool active_vars_compare (const Variables &vars, const Pecos::SurrogateDataVars &sdv) const

  test for exact equality in values between active vars and sdv

Private Attributes

- DiscrepancyCorrection deltaCorr

  manages construction and application of correction functions that are applied to a surrogate model (DataFitSurr or HierarchSurr) in order to reproduce high fidelity data.
- IntIntMap truthIdMap

  map from actualModel/highFidelityModel evaluation ids to DataFitSurrModel/HierarchSurrModel ids
- IntIntMap surrIdMap

  map from approxInterface/lowFidelityModel evaluation ids to DataFitSurrModel/HierarchSurrModel ids
- IntResponseMap cachedApproxRespMap

  map of approximate responses retrieved in derived_synchronize_nowait() that could not be returned since corresponding truth model response portions were still pending.
- IntVariablesMap rawVarsMap

  map of raw continuous variables used by apply_correction(). Model::varsList cannot be used for this purpose since it does not contain lower level variables sets from finite differencing.
- int pointsTotal

  total points the user specified to construct the surrogate
- short pointsManagement

  configuration for points management in build_global()
- String pointReuse

  type of point reuse for approximation builds: `all`, `region` *(default if points file), or* `none` *(default if no points file)*
- String importPointsFile

  file name from `import_build_points_file` *specification*
- String exportPointsFile

  file name from `export_approx_points_file` *specification*
- unsigned short exportFormat

  file export format for variables and approximate responses
- std::ofstream exportFileStream

  output file stream for `export_approx_points_file` *specification*
- String exportVarianceFile

  file name from `export_approx_variance_file` *specification*

- unsigned short exportVarianceFormat

    file export format for variables and approximate response variance
- std::ofstream exportVarianceFileStream

    output file stream for `export_approx_variance_file` *specification*
- Interface approxInterface

    manages the building and subsequent evaluation of the approximations (required for both global and local)
- Model actualModel

    the truth model which provides evaluations for building the surrogate (optional for global, required for local)
- Iterator daceIterator

    selects parameter sets on which to evaluate actualModel in order to generate the necessary data for building global approximations (optional for global since restart data may also be used)

Additional Inherited Members

14.47.1 Detailed Description

Derived model class within the surrogate model branch for managing data fit surrogates (global and local)

The DataFitSurrModel class manages global or local approximations (surrogates that involve data fits) that are used in place of an expensive model. The class contains an approxInterface (required for both global and local) which manages the approximate function evaluations, an actualModel (optional for global, required for local) which provides truth evaluations for building the surrogate, and a daceIterator (optional for global, not used for local) which selects parameter sets on which to evaluate actualModel in order to generate the necessary data for building global approximations.

14.47.2 Member Function Documentation

14.47.2.1 bool finalize_mapping ( ) [protected], [virtual]

Inactive variables must be propagated when a HierarchSurrModel is employed by a sub-iterator (e.g., OUU with MLMC or MLPCE). In current use cases, this can occur once per sub-iterator execution within Model::initialize_-mapping().

Reimplemented from Model.

References DataFitSurrModel::actualModel, Model::finalize_mapping(), and Model::is_null().

14.47.2.2 void update_from_model (const Model & *model*) [protected], [virtual]

update current variables/labels/bounds/targets with data from model

Update values and labels in currentVariables and bound/linear/nonlinear constraints in userDefinedConstraints from variables and constraints data within model.

Reimplemented from SurrogateModel.

References Model::is_null(), SurrogateModel::update_distributions_from_model(), SurrogateModel::update_-response_from_model(), and SurrogateModel::update_variables_from_model().

Referenced by DataFitSurrModel::DataFitSurrModel(), and DataFitSurrModel::update_from_subordinate_model().

14.47.2.3 void derived_evaluate (const ActiveSet & *set*) [protected], [virtual]

Compute the response synchronously using actualModel, approxInterface, or both (mixed case). For the approx-Interface portion, build the approximation if needed, evaluate the approximate response, and apply correction (if active) to the results.

Reimplemented from Model.

References Response::active_set(), DataFitSurrModel::actualModel, SurrogateModel::aggregate_response(), Interface::analysis_components(), DiscrepancyCorrection::apply(), SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, DataFitSurrModel::asv_split_eval(), DataFitSurrModel::build_approximation(), DataFitSurrModel::component_parallel_mode(), DiscrepancyCorrection::compute(), Response::copy(), Model::current_response(), Model::currentResponse, Model::currentVariables, DataFitSurrModel::deltaCorr, Model::eval_tag_prefix(), Model::evalTagPrefix, Model::evaluate(), Interface::evaluation_id(), Model::evaluationsDB, DataFitSurrModel::export_point(), DataFitSurrModel::exportPointsFile, DataFitSurrModel::exportVarianceFile, SurrogateModel::force_rebuild(), Model::hierarchicalTagging, Interface::interface_id(), Model::interfEvaluationsDBState, Interface::map(), Model::modelId, Model::outputLevel, ActiveSet::request_vector(), SurrogateModel::response_combine(), SurrogateModel::responseMode, SurrogateModel::surrModelEvalCntr, Response::update(), and DataFitSurrModel::update_model().

14.47.2.4 void derived_evaluate_nowait (const ActiveSet & *set*) [protected], [virtual]

Compute the response asynchronously using actualModel, approxInterface, or both (mixed case). For the approxInterface portion, build the approximation if needed and evaluate the approximate response in a quasi-asynchronous approach (ApproximationInterface::map() performs the map synchronously and bookkeeps the results for return in derived_synchronize() below).

Reimplemented from Model.

References DataFitSurrModel::actualModel, Interface::analysis_components(), SurrogateModel::approxBuilds, DataFitSurrModel::approxInterface, DataFitSurrModel::asv_split_eval(), DataFitSurrModel::build_approximation(), Variables::copy(), Model::currentResponse, Model::currentVariables, Model::eval_tag_prefix(), Model::evalTagPrefix, Model::evaluate_nowait(), Interface::evaluation_id(), Model::evaluation_id(), Model::evaluationsDB, DataFitSurrModel::exportPointsFile, DataFitSurrModel::exportVarianceFile, SurrogateModel::force_rebuild(), Model::hierarchicalTagging, Interface::interface_id(), Model::interfEvaluationsDBState, Interface::map(), Model::modelId, DataFitSurrModel::rawVarsMap, ActiveSet::request_vector(), SurrogateModel::responseMode, DataFitSurrModel::surrIdMap, SurrogateModel::surrModelEvalCntr, DataFitSurrModel::truthIdMap, and DataFitSurrModel::update_model().

14.47.2.5 const IntResponseMap & derived_synchronize ( ) [protected], [virtual]

Blocking retrieval of asynchronous evaluations from actualModel, approxInterface, or both (mixed case). For the approxInterface portion, apply correction (if active) to each response in the array. derived_synchronize() is designed for the general case where derived_evaluate_nowait() may be inconsistent in its use of actual evaluations, approximate evaluations, or both.

Reimplemented from Model.

References DataFitSurrModel::actualModel, SurrogateModel::aggregate_response(), SurrogateModel::check_key(), DataFitSurrModel::component_parallel_mode(), DiscrepancyCorrection::compute(), DataFitSurrModel::deltaCorr, DataFitSurrModel::derived_synchronize_approx(), Model::outputLevel, Model::rekey_synch(), SurrogateModel::response_combine(), SurrogateModel::responseMode, DataFitSurrModel::surrIdMap, SurrogateModel::surrResponseMap, and DataFitSurrModel::truthIdMap.

14.47.2.6 const IntResponseMap & derived_synchronize_nowait ( ) [protected], [virtual]

Nonblocking retrieval of asynchronous evaluations from actualModel, approxInterface, or both (mixed case). For the approxInterface portion, apply correction (if active) to each response in the map. derived_synchronize_nowait() is designed for the general case where derived_evaluate_nowait() may be inconsistent in its use of actual evals, approx evals, or both.

Reimplemented from Model.

References Dakota::abort_handler(), DataFitSurrModel::actualModel, SurrogateModel::aggregate_response(), DataFitSurrModel::cachedApproxRespMap, DataFitSurrModel::component_parallel_mode(), DiscrepancyCorrection::compute(), DataFitSurrModel::deltaCorr, DataFitSurrModel::derived_synchronize_approx(), Model-

::outputLevel, Model::rekey_synch(), SurrogateModel::response_combine(), SurrogateModel::responseMode, DataFitSurrModel::surrIdMap, SurrogateModel::surrResponseMap, and DataFitSurrModel::truthIdMap.

14.47.2.7 void build_approximation ( ) [protected], [virtual]

Builds the local/multipoint/global approximation using daceIterator/actualModel to generate new data points.

This function constructs a new approximation, discarding any previous data. It constructs any required data for SurrogateData::{vars,resp}Data and does not define an anchor point for SurrogateData::anchor{Vars,Resp}, so is an unconstrained build.

Reimplemented from Model.

References DataFitSurrModel::actualModel, DataFitSurrModel::build_global(), DataFitSurrModel::build_local_-multipoint(), DataFitSurrModel::clear_approx_interface(), Dakota::strbegins(), Model::surrogateType, DataFitSurr-Model::update_global_reference(), DataFitSurrModel::update_local_reference(), and DataFitSurrModel::update_-model().

Referenced by DataFitSurrModel::derived_evaluate(), and DataFitSurrModel::derived_evaluate_nowait().

14.47.2.8 bool build_approximation (const Variables & *vars*, const IntResponsePair & *response_pr*) [protected], [virtual]

Builds the local/multipoint/global approximation using daceIterator/actualModel to generate new data points that augment the passed vars/response anchor point.

This function constructs a new approximation, discarding any previous data. It uses the passed data to populate SurrogateData::anchor{Vars,Resp} and constructs any required data points for SurrogateData::{vars,resp}Data.

Reimplemented from Model.

References DataFitSurrModel::actualModel, DataFitSurrModel::build_global(), DataFitSurrModel::build_local_-multipoint(), Dakota::strbegins(), Model::surrogateType, DataFitSurrModel::update_approx_interface(), DataFitSurr-Model::update_global_reference(), DataFitSurrModel::update_local_reference(), and DataFitSurrModel::update_-model().

14.47.2.9 void rebuild_approximation ( ) [protected], [virtual]

Rebuilds the local/multipoint/global approximation using daceIterator/actualModel to generate an increment of appended data.

This function updates an existing approximation, by appending new data. It does not define an anchor point, so is an unconstrained build.

Reimplemented from Model.

References DataFitSurrModel::actualModel, DataFitSurrModel::build_local_multipoint(), Model::outputLevel, Data-FitSurrModel::rebuild_global(), Dakota::strbegins(), Model::surrogateType, and DataFitSurrModel::update_model().

Referenced by DataFitSurrModel::append_approximation(), DataFitSurrModel::replace_approximation(), and Data-FitSurrModel::update_approximation().

14.47.2.10 void update_approximation (bool *rebuild_flag*) [protected], [virtual]

replaces the approximation data with daceIterator results and rebuilds the approximation if requested

This function populates/replaces SurrogateData::anchor{Vars,Resp} and rebuilds the approximation, if requested. It does not clear other data (i.e., SurrogateData::{vars,resp}Data) and does not update the actualModel with revised bounds, labels, etc. Thus, it updates data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Iterator::all_responses(), Iterator::all_samples(), Iterator::all_variables(), DataFitSurrModel::approxInterface, Iterator::compact_mode(), DataFitSurrModel::daceIterator, Model::outputLevel, DataFitSurrModel::rebuild_approximation(), Model::surrogateType, and Interface::update_approximation().

14.47.2.11 void update_approximation (const Variables & *vars*, const IntResponsePair & *response_pr*, bool *rebuild_flag*) [protected], [virtual]

replaces the anchor point, and rebuilds the approximation if requested

This function populates/replaces SurrogateData::anchor{Vars,Resp} and rebuilds the approximation, if requested. It does not clear other data (i.e., SurrogateData::{vars,resp}Data) and does not update the actualModel with revised bounds, labels, etc. Thus, it updates data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References DataFitSurrModel::approxInterface, Model::outputLevel, DataFitSurrModel::rebuild_approximation(), Model::surrogateType, and Interface::update_approximation().

14.47.2.12 void update_approximation (const VariablesArray & *vars_array*, const IntResponseMap & *resp_map*, bool *rebuild_flag*) [protected], [virtual]

replaces the current points array and rebuilds the approximation if requested

This function populates/replaces SurrogateData::{vars,resp}Data and rebuilds the approximation, if requested. It does not clear other data (i.e., SurrogateData::anchor{Vars,Resp}) and does not update the actualModel with revised bounds, labels, etc. Thus, it updates data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References DataFitSurrModel::approxInterface, Model::outputLevel, DataFitSurrModel::rebuild_approximation(), Model::surrogateType, and Interface::update_approximation().

14.47.2.13 void update_approximation (const RealMatrix & *samples*, const IntResponseMap & *resp_map*, bool *rebuild_flag*) [protected], [virtual]

replaces the current points array and rebuilds the approximation if requested

This function populates/replaces SurrogateData::{vars,resp}Data and rebuilds the approximation, if requested. It does not clear other data (i.e., SurrogateData::anchor{Vars,Resp}) and does not update the actualModel with revised bounds, labels, etc. Thus, it updates data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References DataFitSurrModel::approxInterface, Model::outputLevel, DataFitSurrModel::rebuild_approximation(), Model::surrogateType, and Interface::update_approximation().

14.47.2.14 void append_approximation (bool *rebuild_flag*) [protected], [virtual]

appends daceIterator results to a global approximation and rebuilds it if requested

This function appends all{Samples,Variables,Responses} to SurrogateData::{vars,resp}Data and rebuilds the approximation, if requested.

Reimplemented from Model.

References Iterator::all_responses(), Iterator::all_samples(), Iterator::all_variables(), Interface::append_approximation(), DataFitSurrModel::approxInterface, Iterator::compact_mode(), DataFitSurrModel::daceIterator, Model::outputLevel, DataFitSurrModel::rebuild_approximation(), and Model::surrogateType.

Referenced by DataFitSurrModel::build_global(), DataFitSurrModel::rebuild_global(), and DataFitSurrModel::refine_surrogate().

14.47.2.15 void append_approximation (const Variables & *vars,* const IntResponsePair & *response_pr,* bool *rebuild_flag*) [protected], [virtual]

appends a point to a global approximation and rebuilds it if requested

This function appends one point to SurrogateData::{vars,resp}Data and rebuilds the approximation, if requested. It does not modify other data (i.e., SurrogateData::anchor{Vars,Resp}) and does not update the actualModel with revised bounds, labels, etc. Thus, it appends to data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Interface::append_approximation(), DataFitSurrModel::approxInterface, Model::outputLevel, DataFitSurrModel::rebuild_approximation(), and Model::surrogateType.

14.47.2.16 void append_approximation (const RealMatrix & *samples,* const IntResponseMap & *resp_map,* bool *rebuild_flag*) [protected], [virtual]

appends a matrix of points to a global approximation and rebuilds it if requested

This function appends multiple points to SurrogateData::{vars,resp}Data and rebuilds the approximation, if requested. It does not modify other data (i.e., SurrogateData::anchor{Vars,Resp}) and does not update the actualModel with revised bounds, labels, etc. Thus, it appends to data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Interface::append_approximation(), DataFitSurrModel::approxInterface, Model::outputLevel, DataFitSurrModel::rebuild_approximation(), and Model::surrogateType.

14.47.2.17 void append_approximation (const VariablesArray & *vars_array,* const IntResponseMap & *resp_map,* bool *rebuild_flag*) [protected], [virtual]

appends an array of points to a global approximation and rebuilds it if requested

This function appends multiple points to SurrogateData::{vars,resp}Data and rebuilds the approximation, if requested. It does not modify other data (i.e., SurrogateData::anchor{Vars,Resp}) and does not update the actualModel with revised bounds, labels, etc. Thus, it appends to data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Interface::append_approximation(), DataFitSurrModel::approxInterface, Model::outputLevel, DataFitSurrModel::rebuild_approximation(), and Model::surrogateType.

14.47.2.18 void append_approximation (const IntVariablesMap & *vars_map,* const IntResponseMap & *resp_map,* bool *rebuild_flag*) [protected], [virtual]

appends an map of points to a global approximation and rebuilds it if requested

This function appends multiple points to SurrogateData::{vars,resp}Data and rebuilds the approximation, if requested. It does not modify other data (i.e., SurrogateData::anchor{Vars,Resp}) and does not update the actualModel with revised bounds, labels, etc. Thus, it appends to data from a previous call to build_approximation(), and is not intended to be used in isolation.

Reimplemented from Model.

References Interface::append_approximation(), DataFitSurrModel::approxInterface, Model::outputLevel, DataFitSurrModel::rebuild_approximation(), and Model::surrogateType.

14.47.2.19 void derived_init_communicators (ParLevLIter *pl_iter*, int *max_eval_concurrency*, bool *recurse_flag* = true) [protected], [virtual]

set up actualModel for parallel operations

asynchronous flags need to be initialized for the sub-models. In addition, max_eval_concurrency is the outer level iterator concurrency, not the DACE concurrency that actualModel will see, and recomputing the message_lengths on the sub-model is probably not a bad idea either. Therefore, recompute everything on actualModel using init_-communicators.

Reimplemented from Model.

References DataFitSurrModel::actualModel, DataFitSurrModel::approxInterface, DataFitSurrModel::daceIterator, Model::derivative_concurrency(), ProblemDescDB::get_db_method_node(), ProblemDescDB::get_db_model_-node(), Iterator::init_communicators(), Model::init_communicators(), Iterator::is_null(), Model::is_null(), Iterator-::iterated_model(), Iterator::maximum_evaluation_concurrency(), Iterator::method_id(), Interface::minimum_-points(), Model::model_id(), Model::probDescDB, ProblemDescDB::set_db_list_nodes(), ProblemDescDB::set_-db_method_node(), and ProblemDescDB::set_db_model_nodes().

14.47.2.20 void import_points (unsigned short *tabular_format*, bool *use_var_labels*, bool *active_only*) [private]

optionally read surrogate data points from provided file

Constructor helper to read the points file once, if provided, and then reuse its data as appropriate within build_-global(). Surrogate data imports default to active/inactive variables, but user can override to active only process arrays of data from TabularIO::read_data_tabular() above

References DataFitSurrModel::actualModel, Response::copy(), Variables::copy(), Model::current_response(), Model::current_variables(), Model::currentResponse, Model::currentVariables, Dakota::data_pairs, Param-ResponsePair::eval_id(), Model::evaluation_cache(), DataFitSurrModel::importPointsFile, ParamResponsePair-::interface_id(), Model::interface_id(), Model::is_null(), Model::model_id(), Model::numFns, Model::outputLevel, Model::parallelLib, Model::restart_file(), Variables::total_active(), Variables::tv(), and ParallelLibrary::write_restart().

Referenced by DataFitSurrModel::DataFitSurrModel().

14.47.2.21 void initialize_export ( ) [private]

initialize file stream for exporting surrogate evaluations

Constructor helper to export approximation-based evaluations to a file.

References Model::currentResponse, Model::currentVariables, DataFitSurrModel::exportFileStream, DataFitSurr-Model::exportFormat, DataFitSurrModel::exportPointsFile, DataFitSurrModel::exportVarianceFile, DataFitSurr-Model::exportVarianceFileStream, DataFitSurrModel::exportVarianceFormat, and Response::function_labels().

Referenced by DataFitSurrModel::DataFitSurrModel().

14.47.2.22 void finalize_export ( ) [private]

finalize file stream for exporting surrogate evaluations

Constructor helper to export approximation-based evaluations to a file.

References DataFitSurrModel::exportFileStream, DataFitSurrModel::exportPointsFile, DataFitSurrModel::export-VarianceFile, and DataFitSurrModel::exportVarianceFileStream.

Referenced by DataFitSurrModel::∼DataFitSurrModel().

14.47.2.23 void export_point (int *eval_id*, const Variables & *vars*, const Response & *resp*) [private]

initialize file stream for exporting surrogate evaluations

Constructor helper to export approximation-based evaluations to a file. Exports all variables, so it's clear at what values of inactive it was built at

References DataFitSurrModel::approximation_variances(), Response::copy(), DataFitSurrModel::exportFileStream, DataFitSurrModel::exportFormat, DataFitSurrModel::exportPointsFile, DataFitSurrModel::exportVarianceFile, DataFitSurrModel::exportVarianceFileStream, DataFitSurrModel::exportVarianceFormat, Response::function_values(), DataFitSurrModel::interface_id(), Model::iterator_space_to_user_space(), and Model::recastings().

Referenced by DataFitSurrModel::derived_evaluate(), and DataFitSurrModel::derived_synchronize_approx().

14.47.2.24 void build_local_multipoint ( ) [private]

Builds a local or multipoint approximation using actualModel.

Evaluate the value, gradient, and possibly Hessian needed for a local or multipoint approximation using actualModel.

References Response::active_set(), DataFitSurrModel::actualModel, DataFitSurrModel::asv_inflate_build(), DataFitSurrModel::component_parallel_mode(), Model::continuous_variable_ids(), Model::current_response(), Model::current_variables(), ActiveSet::derivative_vector(), Model::evaluate(), Model::evaluation_id(), Model::hessian_type(), Model::numFns, ActiveSet::request_vector(), Dakota::strbegins(), SurrogateModel::surrogateFnIndices, and Model::surrogateType.

Referenced by DataFitSurrModel::build_approximation(), and DataFitSurrModel::rebuild_approximation().

14.47.2.25 void build_global ( ) [private]

Builds a global approximation using daceIterator.

Determine points to use in building the approximation and then evaluate them on actualModel using daceIterator. Any changes to the bounds should be performed by setting them at a higher level (e.g., SurrBasedOptStrategy).

References Dakota::abort_handler(), DataFitSurrModel::active_vars_compare(), DataFitSurrModel::actualModel, Interface::append_approximation(), DataFitSurrModel::append_approximation(), SurrogateModel::approxBuilds, Interface::approximation_data(), DataFitSurrModel::approxInterface, DataFitSurrModel::autoRefine, DataFitSurrModel::build_approx_interface(), DataFitSurrModel::component_parallel_mode(), DataFitSurrModel::consistent(), Model::currentVariables, Variables::cv(), Model::cv(), DataFitSurrModel::daceIterator, Dakota::data_pairs, Variables::div(), Model::div(), Variables::drv(), Model::drv(), DataFitSurrModel::inside(), Model::interface_id(), Iterator::is_null(), Model::is_null(), Interface::minimum_points(), Iterator::num_samples(), Model::outputLevel, DataFitSurrModel::pointReuse, Model::recastings(), DataFitSurrModel::refine_surrogate(), DataFitSurrModel::required_points(), DataFitSurrModel::run_dace(), Iterator::sampling_reset(), SurrogateModel::surrogateFnIndices, and Model::user_space_to_iterator_space().

Referenced by DataFitSurrModel::build_approximation().

14.47.2.26 void rebuild_global ( ) [private]

Rebuilds a global approximation by generating new data using daceIterator and appending to approxInterface.

Determine points to use in rebuilding the approximation and then evaluate them on actualModel using daceIterator. Assumes data imports/reuse have been handled previously within build_global().

References Dakota::abort_handler(), DataFitSurrModel::append_approximation(), SurrogateModel::approxBuilds, Interface::approximation_data(), DataFitSurrModel::approxInterface, DataFitSurrModel::build_approx_interface(), DataFitSurrModel::component_parallel_mode(), DataFitSurrModel::daceIterator, Interface::formulation_updated(), Iterator::is_null(), Interface::minimum_points(), Model::outputLevel, DataFitSurrModel::required_points(), DataFitSurrModel::run_dace(), Iterator::sampling_reference(), Iterator::sampling_reset(), SurrogateModel::surrogateFnIndices, and Dakota::SZ_MAX.

Referenced by DataFitSurrModel::rebuild_approximation().

14.47.3 Member Data Documentation

14.47.3.1 Model actualModel [private]

the truth model which provides evaluations for building the surrogate (optional for global, required for local)

actualModel is unrestricted in type; arbitrary nestings are possible.

Referenced by DataFitSurrModel::active_model_key(), DataFitSurrModel::asv_inflate_build(), DataFitSurrModel::asv_split_eval(), DataFitSurrModel::build_approx_interface(), DataFitSurrModel::build_approximation(), DataFitSurrModel::build_global(), DataFitSurrModel::build_local_multipoint(), DataFitSurrModel::consistent(), DataFitSurrModel::DataFitSurrModel(), DataFitSurrModel::declare_sources(), DataFitSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate_nowait(), DataFitSurrModel::derived_free_communicators(), DataFitSurrModel::derived_init_communicators(), DataFitSurrModel::derived_init_serial(), DataFitSurrModel::derived_set_communicators(), DataFitSurrModel::derived_subordinate_models(), DataFitSurrModel::derived_synchronize(), DataFitSurrModel::derived_synchronize_nowait(), DataFitSurrModel::estimate_partition_bounds(), DataFitSurrModel::evaluation_cache(), DataFitSurrModel::finalize_mapping(), DataFitSurrModel::fine_grained_evaluation_counters(), DataFitSurrModel::import_points(), DataFitSurrModel::inactive_view(), DataFitSurrModel::initialize_mapping(), DataFitSurrModel::inside(), DataFitSurrModel::nested_acv1_indices(), DataFitSurrModel::nested_acv2_targets(), DataFitSurrModel::nested_variable_mappings(), DataFitSurrModel::primary_response_fn_weights(), DataFitSurrModel::print_evaluation_summary(), DataFitSurrModel::qoi(), DataFitSurrModel::query_distribution_parameter_derivatives(), DataFitSurrModel::rebuild_approximation(), DataFitSurrModel::resize_from_subordinate_model(), DataFitSurrModel::restart_file(), DataFitSurrModel::run_dace(), DataFitSurrModel::serve_run(), DataFitSurrModel::stop_servers(), DataFitSurrModel::surrogate_response_mode(), DataFitSurrModel::truth_model(), DataFitSurrModel::update_from_subordinate_model(), DataFitSurrModel::update_global_reference(), DataFitSurrModel::update_local_reference(), and DataFitSurrModel::warm_start_flag().

The documentation for this class was generated from the following files:

- DataFitSurrModel.hpp
- DataFitSurrModel.cpp

14.48 DataInterface Class Reference

Handle class for interface specification data.

Public Member Functions

- DataInterface ()
  constructor
- DataInterface (const DataInterface &)
  copy constructor
- ∼DataInterface ()
  destructor
- DataInterface & operator= (const DataInterface &)
  assignment operator
- void write (std::ostream &s) const
  write a DataInterface object to an std::ostream
- void read (MPIUnpackBuffer &s)
  read a DataInterface object from a packed MPI buffer
- void write (MPIPackBuffer &s) const
  write a DataInterface object to a packed MPI buffer
- std::shared_ptr< DataInterfaceRep > data_rep ()
  return dataIfaceRep

Static Public Member Functions

- static bool id_compare (const DataInterface &di, const std::string &id)

  compares the idInterface attribute of DataInterface objects

Private Attributes

- std::shared_ptr< DataInterfaceRep > dataIfaceRep

  pointer to the body (handle-body idiom)

Friends

- class **ProblemDescDB**
- class **NIDRProblemDescDB**

14.48.1 Detailed Description

Handle class for interface specification data.

The DataInterface class is used to provide a memory management handle for the data in DataInterfaceRep. It is populated by IDRProblemDescDB::interface_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataInterface objects is maintained in ProblemDescDB::dataInterfaceList, one for each interface specification in an input file.

The documentation for this class was generated from the following files:

- DataInterface.hpp
- DataInterface.cpp

14.49 DataMethod Class Reference

Handle class for method specification data.

Public Member Functions

- DataMethod ()

  constructor
- DataMethod (const DataMethod &)

  copy constructor
- ∼DataMethod ()

  destructor
- DataMethod & operator= (const DataMethod &)

  assignment operator
- void write (std::ostream &s) const

  write a DataMethod object to an std::ostream
- void read (MPIUnpackBuffer &s)

  read a DataMethod object from a packed MPI buffer
- void write (MPIPackBuffer &s) const

  write a DataMethod object to a packed MPI buffer
- std::shared_ptr< DataMethodRep > data_rep ()

  return dataMethodRep

Static Public Member Functions

- static bool id_compare (const DataMethod &dm, const std::string &id)

  compares the idMethod attribute of DataMethod objects

Private Attributes

- std::shared_ptr< DataMethodRep > dataMethodRep

  pointer to the body (handle-body idiom)

Friends

- class **ProblemDescDB**
- class **NIDRProblemDescDB**

14.49.1 Detailed Description

Handle class for method specification data.

The DataMethod class is used to provide a memory management handle for the data in DataMethodRep. It is populated by IDRProblemDescDB::method_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataMethod objects is maintained in ProblemDescDB::dataMethodList, one for each method specification in an input file.

The documentation for this class was generated from the following files:

- DataMethod.hpp
- DataMethod.cpp

14.50 DataMethodRep Class Reference

Body class for method specification data.

Public Member Functions

- ∼DataMethodRep ()

  destructor

Public Attributes

- String idMethod

  string identifier for the method specification data set (from the `id_method` specification in MethodIndControl)
- String modelPointer

  string pointer to the model specification to be used by this method (from the `model_pointer` specification in MethodIndControl)
- String lowFidModelPointer

  string to point to the low fidelity model for Bayesian experimental design
- short methodOutput

  method verbosity control: {SILENT,QUIET,NORMAL,VERBOSE,DEBUG}_OUTPUT (from the `output` specification in MethodIndControl)
- size_t maxIterations

maximum number of iterations allowed for the method (from the `max_iterations` specification in MethodIndControl)

- size_t maxRefineIterations

  maximum number of refinement iterations allowed for a uniform/adaptive refinement approach (from the `max_refinement_iterations` specification in MethodIndControl)

- size_t maxSolverIterations

  maximum number of internal solver iterations allowed for the method (from the `max_solver_iterations` specification in MethodIndControl)

- size_t maxFunctionEvals

  maximum number of function evaluations allowed for the method (from the `max_function_evaluations` specification in MethodIndControl)

- bool speculativeFlag

  flag for use of speculative gradient approaches for maintaining parallel load balance during the line search portion of optimization algorithms (from the `speculative` specification in MethodIndControl)

- bool methodUseDerivsFlag

  flag for usage of derivative data to enhance the computation of surrogate models (PCE/SC expansions, GP models for EGO/EGRA/EGIE) based on the `use_derivatives` specification

- Real constraintTolerance

  tolerance for controlling the amount of infeasibility that is allowed before an active constraint is considered to be violated (from the `constraint_tolerance` specification in MethodIndControl)

- bool methodScaling

  flag indicating scaling status (from the `scaling` specification in MethodIndControl)

- size_t numFinalSolutions

  number of final solutions returned from the iterator

- Real convergenceTolerance

  iteration convergence tolerance for the method (from the `convergence_tolerance` specification in MethodIndControl)

- bool relativeConvMetric

  controls use of convergence tolerance in a relative (true) or absolute (false) context

- short statsMetricMode

  mode of computing statistics metrics used for convergence assessment of multilevel/multifidelity refinement processes: active or combined

- unsigned short methodName

  the method selection: one of the optimizer, least squares, nond, dace, or parameter study methods

- unsigned short subMethod

  enum value for a sub-method type

- String subMethodName

  string identifier for a sub-method name within a multi-option method specification (e.g., from meta-iterators)

- String subModelPointer

  string pointer for a sub-model specification used by a meta-iterator

- String subMethodPointer

  string pointer for a sub-method specification used by a meta-iterator

- int iteratorServers

  number of servers for concurrent iterator parallelism (from the `iterator_servers` specification)

- int procsPerIterator

  number of processors for each concurrent iterator partition (from the `processors_per_iterator` specification)

- short iteratorScheduling

  type of scheduling ({DEFAULT,MASTER,PEER}_SCHEDULING) used in concurrent iterator parallelism (from the `iterator_scheduling` specification)

- StringArray hybridMethodNames

  array of methods for the sequential and collaborative hybrid meta-iterators (from the `method_name_list` specification)

- StringArray hybridModelPointers

array of models for the sequential and collaborative hybrid meta-iterators (from the `model_pointer_list` *specification)*

- StringArray hybridMethodPointers

  array of methods for the sequential and collaborative hybrid meta-iterators (from the `method_pointer_list` *specification)*

- String hybridGlobalMethodName

  global method name for embedded hybrids (from the `global_method_name` *specification)*

- String hybridGlobalModelPointer

  global model pointer for embedded hybrids (from the `global_model_pointer` *specification)*

- String hybridGlobalMethodPointer

  global method pointer for embedded hybrids (from the `global_method_pointer` *specification)*

- String hybridLocalMethodName

  local method name for embedded hybrids (from the `local_method_name` *specification)*

- String hybridLocalModelPointer

  local model pointer for embedded hybrids (from the `local_model_pointer` *specification)*

- String hybridLocalMethodPointer

  local method pointer for embedded hybrids (from the `local_method_pointer` *specification)*

- Real hybridLSProb

  local search probability for embedded hybrids (from the `local_search_probability` *specification)*

- int concurrentRandomJobs

  number of random jobs to perform in the pareto_set and multi_start meta-iterators (from the `random_starts` *and* `random_weight_sets` *specifications)*

- RealVector concurrentParameterSets

  user-specified (i.e., nonrandom) parameter sets to evaluate in the pareto_set and multi_start meta-iterators (from the `starting_points` *and* `weight_sets` *specifications)*

- unsigned short softConvLimit

  number of consecutive iterations with change less than convergenceTolerance required to trigger convergence

- bool surrBasedLocalLayerBypass

  flag to indicate user-specification of a bypass of any/all layerings in evaluating truth response values in SBL.

- RealVector trustRegionInitSize

  initial trust region sizes in the surrogate-based local method (from the `initial_size` *specification in MethodSBL), one size per surrogate model (notes: no trust region for the truth model; sizes are relative values, e.g., 0.1 = 10% of range of global bounds for each variable*

- Real trustRegionMinSize

  minimum trust region size in the surrogate-based local method (from the `minimum_size` *specification in MethodSBL), if the trust region size falls below this threshold the SBL iterations are terminated (note: if kriging is used with SBL, the min trust region size is set to 1.0e-3 in attempt to avoid ill-conditioned matrixes that arise in kriging over small trust regions)*

- Real trustRegionContractTrigger

  trust region minimum improvement level (ratio of actual to predicted decrease in objective fcn) in the surrogate-based local method (from the `contract_threshold` *specification in MethodSBL), the trust region shrinks or is rejected if the ratio is below this value ("eta_1" in the Conn-Gould-Toint trust region book)*

- Real trustRegionExpandTrigger

  trust region sufficient improvement level (ratio of actual to predicted decrease in objective fn) in the surrogate-based local method (from the `expand_threshold` *specification in MethodSBL), the trust region expands if the ratio is above this value ("eta_2" in the Conn-Gould-Toint trust region book)*

- Real trustRegionContract

  trust region contraction factor in the surrogate-based local method (from the `contraction_factor` *specification in MethodSBL)*

- Real trustRegionExpand

  trust region expansion factor in the surrogate-based local method (from the `expansion_factor` *specification in MethodSBL)*

- short surrBasedLocalSubProbObj

SBL approximate subproblem objective: ORIGINAL_PRIMARY, SINGLE_OBJECTIVE, LAGRANGIAN_OBJECTIVE, or AUGMENTED_LAGRANGIAN_OBJECTIVE.

- short surrBasedLocalSubProbCon

  SBL approximate subproblem constraints: NO_CONSTRAINTS, LINEARIZED_CONSTRAINTS, or ORIGINAL_CONSTRAINTS.
- short surrBasedLocalMeritFn

  SBL merit function type: BASIC_PENALTY, ADAPTIVE_PENALTY, BASIC_LAGRANGIAN, or AUGMENTED_LAGRANGIAN.
- short surrBasedLocalAcceptLogic

  SBL iterate acceptance logic: TR_RATIO or FILTER.
- short surrBasedLocalConstrRelax

  SBL constraint relaxation method: NO_RELAX or HOMOTOPY.
- bool surrBasedGlobalReplacePts

  user-specified method for adding points to the set upon which the next surrogate is based in the `surrogate_based_global` *method.*
- String dlDetails

  string of options for a dynamically linked solver
- void ∗ dlLib

  handle to dynamically loaded library
- int verifyLevel

  the `verify_level` *specification in MethodNPSOLDC*
- Real functionPrecision

  the `function_precision` *specification in MethodNPSOLDC and the* `EPSILON` *specification in NOMAD*
- Real lineSearchTolerance

  the `linesearch_tolerance` *specification in MethodNPSOLDC*
- Real absConvTol

  absolute function convergence tolerance
- Real xConvTol

  x-convergence tolerance
- Real singConvTol

  singular convergence tolerance
- Real singRadius

  radius for singular convergence test
- Real falseConvTol

  false-convergence tolerance
- Real initTRRadius

  initial trust radius
- int covarianceType

  kind of covariance required
- bool regressDiag

  whether to print the regression diagnostic vector
- String searchMethod

  the `search_method` *specification for Newton and nonlinear interior-point methods in MethodOPTPPDC*
- Real gradientTolerance

  the `gradient_tolerance` *specification in MethodOPTPPDC*
- Real maxStep

  the `max_step` *specification in MethodOPTPPDC*
- short meritFn

  the `merit_function` *specification for nonlinear interior-point methods in MethodOPTPPDC*
- Real stepLenToBoundary

  the `steplength_to_boundary` *specification for nonlinear interior-point methods in MethodOPTPPDC*

- Real centeringParam

    the `centering_parameter` *specification for nonlinear interior-point methods in MethodOPTPPDC*
- int searchSchemeSize

    the `search_scheme_size` *specification for PDS methods in MethodOPTPPDC*
- Real initStepLength

    the `initStepLength` *choice for nonlinearly constrained APPS in MethodAPPSDC*
- Real contractStepLength

    the `contractStepLength` *choice for nonlinearly constrained APPS in MethodAPPSDC*
- Real threshStepLength

    the `threshStepLength` *choice for nonlinearly constrained APPS in MethodAPPSDC*
- String meritFunction

    the `meritFunction` *choice for nonlinearly constrained APPS in MethodAPPSDC*
- Real constrPenalty

    the `constrPenalty` *choice for nonlinearly constrained APPS in MethodAPPSDC*
- Real smoothFactor

    the initial `smoothFactor` *value for nonlinearly constrained APPS in MethodAPPSDC*
- Real constraintPenalty

    the initial `constraint_penalty` *for COLINY methods in MethodAPPS, MethodSCOLIBDIR, MethodSCOLIBPS, MethodSCOLIBSW and MethodSCOLIBEA*
- bool constantPenalty

    the `constant_penalty` *flag for COLINY methods in MethodSCOLIBPS and MethodSCOLIBSW*
- Real globalBalanceParam

    the `global_balance_parameter` *for the DIRECT method in MethodSCOLIBDIR*
- Real localBalanceParam

    the `local_balance_parameter` *for the DIRECT method in MethodSCOLIBDIR*
- Real maxBoxSize

    the `max_boxsize_limit` *for the DIRECT method in MethodSCOLIBDIR*
- Real minBoxSize

    the `min_boxsize_limit` *for the DIRECT method in MethodSCOLIBDIR and MethodNCSUDC*
- String boxDivision

    the `division` *setting (*`major_dimension` *or* `all_dimensions`*) for the DIRECT method in MethodSCOLIB-DIR*
- bool mutationAdaptive

    the `non_adaptive` *specification for the coliny_ea method in MethodSCOLIBEA*
- bool showMiscOptions

    the `show_misc_options` *specification in MethodSCOLIBDC*
- StringArray miscOptions

    the `misc_options` *specification in MethodSCOLIBDC*
- Real solnTarget

    the `solution_target` *specification in MethodSCOLIBDC*
- Real crossoverRate

    the `crossover_rate` *specification for EA methods in MethodSCOLIBEA*
- Real mutationRate

    the `mutation_rate` *specification for EA methods in MethodSCOLIBEA*
- Real mutationScale

    the `mutation_scale` *specification for EA methods in MethodSCOLIBEA*
- Real mutationMinScale

    the `min_scale` *specification for mutation in EA methods in MethodSCOLIBEA*
- Real initDelta

    the `initial_delta` *specification for APPS/COBYLA/PS/SW methods in MethodAPPS, MethodSCOLIBCOB, MethodSCOLIBPS, and MethodSCOLIBSW*

- Real threshDelta

    the `variable_tolerance` *specification for APPS/COBYLA/PS/SW methods in MethodAPPS, MethodSCOLIB-COB, MethodSCOLIBPS, and MethodSCOLIBSW*

- Real contractFactor

    the `contraction_factor` *specification for APPS/PS/SW methods in MethodAPPS, MethodSCOLIBPS, and MethodSCOLIBSW*

- int newSolnsGenerated

    the `new_solutions_generated` *specification for GA/EPSA methods in MethodSCOLIBEA*

- int numberRetained

    the integer assignment to random, chc, or elitist in the `replacement_type` *specification for GA/EPSA methods in MethodSCOLIBEA*

- bool expansionFlag

    the `no_expansion` *specification for APPS/PS/SW methods in MethodAPPS, MethodSCOLIBPS, and MethodSC-OLIBSW*

- int expandAfterSuccess

    the `expand_after_success` *specification for PS/SW methods in MethodSCOLIBPS and MethodSCOLIBSW*

- int contractAfterFail

    the `contract_after_failure` *specification for the SW method in MethodSCOLIBSW*

- int mutationRange

    the `mutation_range` *specification for the pga_int method in MethodSCOLIBEA*

- int totalPatternSize

    the `total_pattern_size` *specification for PS methods in MethodSCOLIBPS*

- bool randomizeOrderFlag

    the `stochastic` *specification for the PS method in MethodSCOLIBPS*

- String selectionPressure

    the `fitness_type` *specification for EA methods in MethodSCOLIBEA*

- String replacementType

    the `replacement_type` *specification for EA methods in MethodSCOLIBEA*

- String crossoverType

    the `crossover_type` *specification for EA methods in MethodSCOLIBEA*

- String mutationType

    the `mutation_type` *specification for EA methods in MethodSCOLIBEA*

- String exploratoryMoves

    the `exploratory_moves` *specification for the PS method in MethodSCOLIBPS*

- String patternBasis

    the `pattern_basis` *specification for APPS/PS methods in MethodAPPS and MethodSCOLIBPS*

- String betaSolverName

    beta solvers don't need documentation

- short evalSynchronize

    the `synchronization` *setting for parallel pattern search methods in MethodSCOLIBPS and MethodAPPS*

- size_t numCrossPoints

    The number of crossover points or multi-point schemes.

- size_t numParents

    The number of parents to use in a crossover operation.

- size_t numOffspring

    The number of children to produce in a crossover operation.

- String fitnessType

    the fitness assessment operator to use.

- String convergenceType

    The means by which this JEGA should converge.

- Real percentChange

The minimum percent change before convergence for a fitness tracker converger.
- size_t numGenerations

  The number of generations over which a fitness tracker converger should track.
- Real fitnessLimit

  The cutoff value for survival in fitness limiting selectors (e.g., below_limit selector).
- Real shrinkagePercent

  The minimum percentage of the requested number of selections that must take place on each call to the selector (0, 1).
- String nichingType

  The niching type.
- RealVector nicheVector

  The discretization percentage along each objective.
- size_t numDesigns

  The maximum number of designs to keep when using the max_designs nicher.
- String postProcessorType

  The post processor type.
- RealVector distanceVector

  The discretization percentage along each objective.
- String initializationType

  The means by which the JEGA should initialize the population.
- String flatFile

  The filename to use for initialization.
- String logFile

  The filename to use for logging.
- int populationSize

  the `population_size` specification for GA methods in MethodSCOLIBEA
- bool printPopFlag

  The `print_each_pop` flag to set the printing of the population at each generation.
- Real volBoxSize

  the `volume_boxsize_limit` for the DIRECT method in MethodNCSUDC
- int numSymbols

  the `symbols` specification for DACE methods
- bool mainEffectsFlag

  the `main_effects` specification for sampling methods in MethodDDACE)
- bool latinizeFlag

  the `latinize` specification for FSU QMC and CVT methods in MethodFSUDACE
- bool volQualityFlag

  the `quality_metrics` specification for sampling methods (FSU QMC and CVT methods in MethodFSUDACE)
- IntVector sequenceStart

  the `sequenceStart` specification in MethodFSUDACE
- IntVector sequenceLeap

  the `sequenceLeap` specification in MethodFSUDACE
- IntVector primeBase

  the `primeBase` specification in MethodFSUDACE
- int numTrials

  the `numTrials` specification in MethodFSUDACE
- String trialType

  the `trial_type` specification in MethodFSUDACE
- int randomSeed

  the `seed` specification for COLINY, NonD, & DACE methods
- SizetArray randomSeedSeq

the `seed_sequence` specification for multilevel UQ methods

- RealVector scalarizationRespCoeffs

    the `coefficient` mapping for the scalarization term for multilevel UQ methods

- Real initMeshSize

    the `initMeshSize` choice for NOMAD in MethodNOMADDC

- Real minMeshSize

    the `minMeshSize` choice for NOMAD in MethodNOMADDC

- String historyFile

    the `HISTORY_FILE` specification for NOMAD

- String displayFormat

    the `DISPLAY_STATS` specification for NOMAD

- Real vns

    the `VNS` specification for NOMAD

- int neighborOrder

    the `NEIGHBOR_ORDER` specification for NOMAD

- bool showAllEval

    the `DISPLAY_ALL_EVAL` specification for NOMAD

- String useSurrogate

    the `HAS_SGTE` specification for NOMAD

- int maxCrossIterations

    maximum number of cross iterations

- Real solverTol

    optimization tolerance for FT regression

- Real solverRoundingTol

    Rounding tolerance for FT regression.

- Real statsRoundingTol

    arithmetic (rounding) tolerance for FT sums and products

- unsigned short startOrder

    starting polynomial order

- unsigned short kickOrder

    polynomial order increment when adapting

- unsigned short maxOrder

    maximum order of basis polynomials

- bool adaptOrder

    whether or not to adapt order by cross validation

- size_t startRank

    starting rank

- size_t kickRank

    rank increment when adapting

- size_t maxRank

    maximum rank

- bool adaptRank

    whether or not to adapt rank

- size_t maxCVRankCandidates

    maximum number of cross-validation candidates for adaptRank

- unsigned short maxCVOrderCandidates

    maximum number of cross-validation candidates for adaptOrder

- short c3AdvanceType

    quantity to increment (start rank, start order, max rank, max order, max rank + max order) for FT (uniform) p-refinement

- UShortArray startOrderSeq

starting polynomial order

- SizetArray startRankSeq

  starting rank
- int numSamples

  the `samples` *specification for NonD & DACE methods*
- bool fixedSeedFlag

  flag for fixing the value of the seed among different NonD/DACE sample sets. This results in the use of the same sampling stencil/pattern throughout an execution with repeated sampling.
- bool fixedSequenceFlag

  flag for fixing the sequence for Halton or Hammersley QMC sample sets. This results in the use of the same sampling stencil/pattern throughout an execution with repeated sampling.
- bool vbdFlag

  the `var_based_decomp` *specification for a variety of sampling methods*
- Real vbdDropTolerance

  the `var_based_decomp` *tolerance for omitting index output*
- bool backfillFlag

  the `backfill` *option allows one to augment in LHS sample by enforcing the addition of unique discrete variables to the sample*
- bool pcaFlag

  Flag to specify the calculation of principal components when using LHS.
- Real percentVarianceExplained

  The percentage of variance explained by using a truncated number of principal components in PCA.
- bool wilksFlag

  Flag to specify use of Wilks formula to calculate num samples.
- unsigned short wilksOrder

  Wilks order parameter.
- Real wilksConfidenceLevel

  Wilks confidence interval parameter.
- short wilksSidedInterval

  Wilks sided interval type.
- bool respScalingFlag

  flag to indicate bounds-based scaling of current response data set prior to build in surrogate-based methods; important for ML/MF data fits of decaying discrepancy data using regression with absolute tolerances
- unsigned short vbdOrder

  a sub-specification of vbdFlag: interaction order limit for calculation/output of component VBD indices
- short covarianceControl

  restrict the calculation of a full response covariance matrix for high dimensional outputs: {DEFAULT,DIAGONAL,FULL}_COVARIANCE
- String rngName

  the `basic` *random-number generator for NonD*
- short refinementType

  refinement type for stochastic expansions from dimension refinement keyword group
- short refinementControl

  refinement control for stochastic expansions from dimension refinement keyword group
- short nestingOverride

  override for default point nesting policy: NO_NESTING_OVERRIDE, NESTED, or NON_NESTED
- short growthOverride

  override for default point growth restriction policy: NO_GROWTH_OVERRIDE, RESTRICTED, or UNRESTRICTED
- short expansionType

  enumeration for u-space type that defines u-space variable targets for probability space transformations: EXTENDED_U (default), ASKEY_U, PARTIAL_ASKEY_U, STD_NORMAL_U, or STD_UNIFORM_U
- bool piecewiseBasis

boolean indicating presence of `piecewise` keyword

- short expansionBasisType

    enumeration for type of basis in sparse grid interpolation (Pecos::{NODAL,HIERARCHICAL}_INTERPOLANT) or regression (Pecos::{TENSOR_PRODUCT,TOTAL_ORDER,ADAPTED}_BASIS).

- UShortArray quadratureOrderSeq

    the `quadrature_order_sequence` specification in MethodNonDPCE and MethodNonDSC

- UShortArray sparseGridLevelSeq

    the `sparse_grid_level_sequence` specification in MethodNonDPCE and MethodNonDSC

- UShortArray expansionOrderSeq

    the `expansion_order_sequence` specification in MethodNonDPCE

- SizetArray collocationPointsSeq

    the `collocation_points_sequence` specification in MethodNonDPCE

- SizetArray expansionSamplesSeq

    the `expansion_samples_sequence` specification in MethodNonDPCE

- unsigned short quadratureOrder

    the `quadrature_order` specification in MethodNonDPCE and MethodNonDSC

- unsigned short sparseGridLevel

    the `sparse_grid_level` specification in MethodNonDPCE and MethodNonDSC

- unsigned short expansionOrder

    the `expansion_order` specification in MethodNonDPCE

- size_t collocationPoints

    the `collocation_points` specification in MethodNonDPCE

- size_t expansionSamples

    the `expansion_samples` specification in MethodNonDPCE

- RealVector anisoDimPref

    the `dimension_preference` specification for tensor and sparse grids and expansion orders in MethodNonDPCE and MethodNonDSC

- unsigned short cubIntOrder

    the `cubature_integrand` specification in MethodNonDPCE

- Real collocationRatio

    the `collocation_ratio` specification in MethodNonDPCE

- Real collocRatioTermsOrder

    order applied to the number of expansion terms when applying or computing the collocation ratio within regression PCE; based on the `ratio_order` specification in MethodNonDPCE

- short regressionType

    type of regression: LS, OMP, BP, BPDN, LARS, or LASSO

- short lsRegressionType

    type of least squares regression: SVD or EQ_CON_QR

- RealVector regressionNoiseTol

    noise tolerance(s) for OMP, BPDN, LARS, and LASSO

- Real regressionL2Penalty

    L2 regression penalty for a variant of LASSO known as the elastic net method (default of 0 gives standard LASSO)

- bool crossValidation

    flag indicating the use of cross-validation across expansion orders (given a prescribed maximum order) and, for some methods, noise tolerances

- bool crossValidNoiseOnly

    flag indicating the restriction of cross-validation to estimate only the most effective noise tolerance; used to reduce cost from performing CV over both noise tolerances and expansion orders

- unsigned short adaptedBasisAdvancements

    initial grid level for the ADAPTED_BASIS_EXPANDING_FRONT approach to defining the candidate basis for sparse recovery (compressed sensing)

- bool normalizedCoeffs

flag indicating the output of PCE coefficients corresponding to normalized basis polynomials

- String pointReuse

  allows PCE construction to reuse points from previous sample sets or data import using the `reuse_points` *specification in MethodNonDPCE*

- bool tensorGridFlag

  flag for usage of a sub-sampled set of tensor-product grid points within regression PCE; based on the `tensor_grid` *specification in MethodNonDPCE*

- UShortArray tensorGridOrder

  order of tensor-product grid points that are sub-sampled within orthogonal least interpolation PCE; based on the `tensor_grid` *specification in MethodNonDPCE*

- String importExpansionFile

  the `import_expansion_file` *specification in MethodNonDPCE*

- String exportExpansionFile

  the `export_expansion_file` *specification in MethodNonDPCE*

- unsigned short sampleType

  the `sample_type` *specification in MethodNonDMC, MethodNonDPCE, and MethodNonDSC*

- bool dOptimal

  whether to generate D-optimal designs

- size_t numCandidateDesigns

  number of candidate designss in D-optimal design selection

- String reliabilityIntegration

  the `first_order` *or* `second_order` *integration selection in MethodNonDLocalRel*

- unsigned short integrationRefine

  the `import`*,* `adapt_import`*, or* `mm_adapt_import` *integration refinement selection in MethodNonDLocalRel, MethodNonDPCE, and MethodNonDSC*

- IntVector refineSamples

  Sequence of refinement samples, e.g., the size of the batch (e.g. number of supplemental points added) to be added to be added to the build points for an emulator at each iteration.

- unsigned short optSubProbSolver

  the method used for solving an optimization sub-problem (e.g., pre-solve for the MAP point)

- unsigned short numericalSolveMode

  approach for overriding an analytic solution based on simplifying assumptions that might be violated, suggesting a fallback approach, or lacking robustness, suggesting an optional override replacement

- SizetArray pilotSamples

  the `pilot_samples` *selection in MethodMultilevelMC*

- short ensembleSampSolnMode

  the `solution_mode` *selection for ML/MF sampling methods*

- bool truthPilotConstraint

  the `truth_fixed_by_pilot` *flag for ACV methods*

- short allocationTarget

  the `allocationTarget` *selection in MethodMultilevelMC*

- bool useTargetVarianceOptimizationFlag

  the `useTargetVarianceOptimizationFlag` *selection in MethodMultilevelMC*

- short qoiAggregation

  the |c qoi_aggregation_norm selection in MethodMultilevelMC

- short convergenceToleranceType

  the |c convergence_tolerance_type selection in MethodMultilevelMC

- short convergenceToleranceTarget

  the |c convergence_tolerance_type selection in MethodMultilevelMC

- short multilevAllocControl

  the `allocation_control` *selection in MethodMultilevelPCE*

- Real multilevEstimatorRate

the `estimator_rate` selection in MethodMultilevelPCE

- short multilevDiscrepEmulation

  type of discrepancy emulation in multilevel methods: distinct or recursive
- short finalStatsType

  specification of the type of final statistics in MethodNonD
- short finalMomentsType

  the `final_moments` specification in MethodNonD, subordinate to the type of final statistics
- short distributionType

  the `distribution` `cumulative` or `complementary` specification in MethodNonD
- short responseLevelTarget

  the `compute` `probabilities`, `reliabilities`, or `gen_reliabilities` specification in MethodNonD
- short responseLevelTargetReduce

  the `system` `series` or `parallel` specification in MethodNonD
- RealVectorArray responseLevels

  the `response_levels` specification in MethodNonD
- RealVectorArray probabilityLevels

  the `probability_levels` specification in MethodNonD
- RealVectorArray reliabilityLevels

  the `reliability_levels` specification in MethodNonD
- RealVectorArray genReliabilityLevels

  the `gen_reliability_levels` specification in MethodNonD
- int chainSamples

  the number of MCMC chain samples
- int buildSamples

  the number of samples to construct an emulator, e.g., for Bayesian calibration methods
- int samplesOnEmulator

  number of samples to perform on emulator
- int emulatorOrder

  The total order to be used in construction of a VPS surrogate.
- short emulatorType

  the `emulator` specification in MethodNonDBayesCalib
- String mcmcType

  the `mcmc` type specification in MethodNonDBayesCalib
- bool standardizedSpace

  use of standardized probability spaces for MCMC within Bayesian inference
- bool adaptPosteriorRefine

  flag indicating adaptive refinement of the emulator in regions of high posterior probability
- bool logitTransform

  flag indicating user activation of logit transform option within QUESO
- bool gpmsaNormalize

  whether to apply GPMSA-internal normalization
- bool posteriorStatsKL

  flag indicating the calculation of KL divergence between prior and posterior in Bayesian methods
- bool posteriorStatsMutual

  flag indicating the calculation of mutual information between prior and posterior in Bayesian methods
- bool posteriorStatsKDE

  flag indicating calculation of kernel density estimate of posterior distributions
- bool chainDiagnostics

  flag indicating calculation of chain diagnostics
- bool chainDiagnosticsCI

  flag indicating calculation of confidence intervals as a chain diagnositc

- bool modelEvidence

    flag indicating calculation of the evidence of the model
- bool modelEvidMC

    flag indicating use of Monte Carlo approximation for evidence calc.
- int evidenceSamples

    number of prior samples to use in model evidence calculation
- bool modelEvidLaplace

    flag indicating use of Laplace approximation for evidence calc.
- String proposalCovType

    the type of proposal covariance: user, derivatives, or prior
- Real priorPropCovMult

    optional multiplier for prior-based proposal covariance
- int proposalCovUpdatePeriod

    number of samples after which to update the proposal covariance from misfit Hessian (using residual values and derivatives)
- String proposalCovInputType

    the format of proposal covariance input: diagonal or matrix
- RealVector proposalCovData

    raw list of real data for the proposal covariance
- String proposalCovFile

    file from which to read proposal covariance in diagonal or matrix format
- String advancedOptionsFilename

    file containing advanced ROL option overrides
- String quesoOptionsFilename

    file containing advanced QUESO option overrides
- String fitnessMetricType

    the `fitness` metric type specification in MethodNonDAdaptive
- String batchSelectionType

    the `batch` selection type specification in MethodNonDAdaptive
- String lipschitzType

    the `Lipschitz` type specification in MethodNonDPOFDarts (e.g. either local or global estimation)
- unsigned short calibrateErrorMode

    calibration mode for observation error multipliers (CALIBRATE_∗)
- RealVector hyperPriorAlphas

    hyperparameters inverse gamma prior alphas
- RealVector hyperPriorBetas

    hyperparameters inverse gamma prior alphas
- int burnInSamples

    number of MCMC samples to discard from acceptance chain
- int subSamplingPeriod

    period or skip in post-processing the acceptance chain
- bool calModelDiscrepancy

    flag to calculate model discrepancy
- size_t numPredConfigs

    number of prediction configurations at which to calculate model discrepancy
- RealVector predictionConfigList

    list of prediction configurations at which to calculate model discrepancy
- String importPredConfigs

    whether to import prediction configurations at which to calculate model discrepancy
- unsigned short importPredConfigFormat

    tabular format for prediction configurations import file

- String modelDiscrepancyType

    type of model discrepancy emulation
- short polynomialOrder

    polynomial order for model discrepancy calculations: either gaussian process trend order or polynomial basis order
- String exportCorrModelFile

    specify the name of file to which corrected model (model+discrepancy) calculations are output
- unsigned short exportCorrModelFormat

    tabular format for corrected model (model+discrepancy) export file
- String exportCorrVarFile

    specify the name of file to which corrected model variance calculations are output
- unsigned short exportCorrVarFormat

    tabular format for corrected model variance export file
- String exportDiscrepFile

    specify the name of file to which discrepancy calculations are output
- unsigned short exportDiscrepFormat

    tabular format for model discrepancy export file
- bool adaptExpDesign

    whether to perform adaptive Bayesian design of experiments
- String importCandPtsFile

    whether to import candidate design points for adaptive Bayesian experimental design
- unsigned short importCandFormat

    tabular format for the candidate design points import file
- size_t numCandidates

    number of candidate designs for adaptive Bayesian experimental design
- int maxHifiEvals

    maximum number of highfidelity model runs to be used for adaptive Bayesian experimental design
- int batchSize

    number of optimal designs selected per iteration of experimental design algorithm; also number of concurrent GP refinement points for EGO
- int batchSizeExplore

    portion of batchSize earmarked for exploration rather than acquisition
- bool mutualInfoKSG2

    indicate that the KSG2 algorithm is to be employed in the calculation of the mutual information
- int numChains

    number of concurrent chains
- int numCR

    number of CR-factors
- int crossoverChainPairs

    number of crossover chain pairs
- Real grThreshold

    threshold for the Gelmin-Rubin statistic
- int jumpStep

    how often to perform a long jump in generations
- int numPushforwardSamples

    Number of samples from the prior that is pushed forward through the model to obtain the initial set of pushforward samples.
- String dataDistType

    the type of data distribution: kde, or gaussian
- String dataDistCovInputType

    the format of data distribution gaussian covariance input: diagonal or matrix
- RealVector dataDistMeans

raw list of real data for the data distribution gaussian means

- RealVector dataDistCovariance

  raw list of real data for the data distribution gaussian covariance
- String dataDistFile

  file from which to read data distribution data (covariance or samples)
- String posteriorDensityExportFilename

  The filename of the export file containing an arbitrary set of samples and their corresponding density values.
- String posteriorSamplesExportFilename

  The filename of the export file containing samples from the posterior and their corresponding density values.
- String posteriorSamplesImportFilename

  The filename of the import file containing samples at which the posterior will be evaluated.
- bool generatePosteriorSamples

  Flag specifying whether to generate random samples from the posterior.
- bool evaluatePosteriorDensity

  Flag specifying whether to evaluate the posterior density at a set of samples.
- RealVector finalPoint

  the `final_point` specification in MethodPSVPS
- RealVector stepVector

  the `step_vector` specification in MethodPSVPS and MethodPSCPS
- int numSteps

  the `num_steps` specification in MethodPSVPS
- IntVector stepsPerVariable

  the `deltas_per_variable` specification in MethodPSCPS
- RealVector listOfPoints

  the `list_of_points` specification in MethodPSLPS
- String pstudyFilename

  the `import_points_file` spec for a file-based parameter study
- unsigned short pstudyFileFormat

  tabular format for the parameter study points file
- bool pstudyFileActive

  whether to import active variables only
- UShortArray varPartitions

  the `partitions` specification for PStudy method in MethodPSMPS
- Real refinementRate

  rate of mesh refinement in Richardson extrapolation
- String importBuildPtsFile

  the file name from the `import_build_points_file` specification
- unsigned short importBuildFormat

  tabular format for the build point import file
- bool importBuildActive

  whether to import active variables only
- String importApproxPtsFile

  the file name from the `import_approx_points_file` specification
- unsigned short importApproxFormat

  tabular format for the approx point import file
- bool importApproxActive

  whether to import active variables only
- String exportApproxPtsFile

  the file name from the `export_approx_points_file` specification
- unsigned short exportApproxFormat

  tabular format for the approx point export file

- String exportMCMCPtsFile

    the file name from the `export_mcmc_points_file` *specification*
- bool exportSampleSeqFlag

    flag for exporting the sequence of sample increments within multilevel sampling from the `export_sample_-sequence` *specification*
- unsigned short exportSamplesFormat

    tabular format for the MCMC chain and MLMC sample sequence exports
- bool exportSurrogate

    Option to turn on surrogate model export (export_model)
- String modelExportPrefix

    the filename prefix for export_model
- unsigned short modelExportFormat

    Format selection for export_model.

Private Member Functions

- DataMethodRep ()

    constructor
- void write (std::ostream &s) const

    write a DataInterfaceRep object to an std::ostream
- void read (MPIUnpackBuffer &s)

    read a DataInterfaceRep object from a packed MPI buffer
- void write (MPIPackBuffer &s) const

    write a DataInterfaceRep object to a packed MPI buffer

Friends

- class DataMethod

    the handle class can access attributes of the body class directly

14.50.1 Detailed Description

Body class for method specification data.

The DataMethodRep class is used to contain the data from a method keyword specification. Default values are managed in the DataMethodRep constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::dataMethodList is private.

The documentation for this class was generated from the following files:

- DataMethod.hpp
- DataMethod.cpp

14.51 DataModel Class Reference

Handle class for model specification data.

Public Member Functions

- DataModel ()

  constructor
- DataModel (const DataModel &)

  copy constructor
- ∼DataModel ()

  destructor
- DataModel & operator= (const DataModel &)

  assignment operator
- void write (std::ostream &s) const

  write a DataModel object to an std::ostream
- void read (MPIUnpackBuffer &s)

  read a DataModel object from a packed MPI buffer
- void write (MPIPackBuffer &s) const

  write a DataModel object to a packed MPI buffer
- std::shared_ptr< DataModelRep > data_rep ()

  return dataModelRep

Static Public Member Functions

- static bool id_compare (const DataModel &dm, const std::string &id)

  compares the idModel attribute of DataModel objects

Private Attributes

- std::shared_ptr< DataModelRep > dataModelRep

  pointer to the body (handle-body idiom)

Friends

- class **ProblemDescDB**
- class **NIDRProblemDescDB**

14.51.1 Detailed Description

Handle class for model specification data.

The DataModel class is used to provide a memory management handle for the data in DataModelRep. It is populated by IDRProblemDescDB::model_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataModel objects is maintained in ProblemDescDB::dataModelList, one for each model specification in an input file.

The documentation for this class was generated from the following files:

- DataModel.hpp
- DataModel.cpp

14.52 DataModelRep Class Reference

Body class for model specification data.

Public Member Functions

- ∼DataModelRep ()

  destructor

Public Attributes

- String idModel

  string identifier for the model specification data set (from the `id_model` *specification in ModelIndControl)*
- String modelType

  model type selection: single, surrogate, or nested (from the model type specification in ModelIndControl)
- String variablesPointer

  string pointer to the variables specification to be used by this model (from the `variables_pointer` *specification in ModelIndControl)*
- String interfacePointer

  string pointer to the interface specification to be used by this model (from the `interface_pointer` *specification in ModelSingle and the* `optional_interface_pointer` *specification in ModelNested)*
- String responsesPointer

  string pointer to the responses specification to be used by this model (from the `responses_pointer` *specification in ModelIndControl)*
- bool hierarchicalTags

  whether this model and its children will add hierarchy-based tags to eval ids
- String subMethodPointer

  pointer to a sub-iterator used for global approximations (from the `dace_method_pointer` *specification in Model-SurrG) or by nested models (from the* `sub_method_pointer` *specification in ModelNested)*
- String solutionLevelControl

  (state) variable identifier that defines a set or range of solution level controls (space/time discretization levels, iterative convergence tolerances, etc.) for defining a secondary hierarchy of fidelity within the scope of a single model form (from `solution_level_control` *specification; see also* `ordered_model_fidelities`*)*
- RealVector solutionLevelCost

  array of relative simulation costs corresponding to each of the solution levels (from `solution_level_cost` *specification; see also* `solution_level_control`*); a scalar input is interpreted as a constant cost multiplier to be applied recursively*
- String costRecoveryMetadata

  identifier for response metadata that returns the incurred cost of a simulation execution. This online recovery option (typically averaged over a pilot sample) can replace the need for a priori specification of solutionLevelCost.
- SizetSet surrogateFnIndices

  array specifying the response function set that is approximated
- String surrogateType

  the selected surrogate type: local_taylor, multipoint_tana, global_(neural_network,mars,orthogonal_polynomial,gaussian, polynomial,kriging), or hierarchical
- String truthModelPointer

  pointer to the model specification for constructing the truth model used in constructing surrogates
- StringArray ensembleModelPointers

  an ordered (low to high) or unordered (peer) set of model pointers corresponding to a ensemble of modeling fidelities (from the `ordered_model_fidelities` *specification in ModelSurrH or the* `unordered_model_fidelities` *specification in ModelSurrNonH)*
- int pointsTotal

  user-specified lower bound on total points with which to build the model (if reuse_points $<$ pointsTotal, new samples will make up the difference)
- short pointsManagement

  points management configuration for DataFitSurrModel: DEFAULT_POINTS, MINIMUM_POINTS, or RECOMMENDED_POINTS
- String approxPointReuse

sample reuse selection for building global approximations: none, all, region, or file (from the `reuse_samples` *specification in ModelSurrG)*

- String importBuildPtsFile

  the file name from the `import_build_points_file` *specification in ModelSurrG*
- unsigned short importBuildFormat

  tabular format for the build point import file
- bool importUseVariableLabels

  whether to parse/validate variable labels from header
- bool importBuildActive

  whether to import active variables only
- String exportApproxPtsFile

  the file name from the `export_approx_points_file` *specification in ModelSurrG*
- unsigned short exportApproxFormat

  tabular format for the approx point export file
- String exportApproxVarianceFile

  filename for surrogate variance evaluation export
- unsigned short exportApproxVarianceFormat

  tabular format for the approx variance export file
- bool exportSurrogate

  Option to turn on surrogate model export (export_model)
- String modelExportPrefix

  the filename prefix for export_model
- unsigned short modelExportFormat

  Format selection for export_model.
- bool importSurrogate

  Option to turn on surrogate model import (import_model)
- String modelImportPrefix

  the filename prefix for import_model
- unsigned short modelImportFormat

  Format selection for import_model.
- short approxCorrectionType

  correction type for global and hierarchical approximations: NO_CORRECTION, ADDITIVE_CORRECTION, MULTIPLICATIVE_CORRECTION, or COMBINED_CORRECTION (from the `correction` *specification in ModelSurrG and ModelSurrH)*
- short approxCorrectionOrder

  correction order for global and hierarchical approximations: 0, 1, or 2 (from the `correction` *specification in ModelSurrG and ModelSurrH)*
- bool modelUseDerivsFlag

  flags the use of derivatives in building global approximations (from the `use_derivatives` *specification in ModelSurrG)*
- bool respScalingFlag

  flag to indicate bounds-based scaling of current response data set prior to surrogate build; important for data fits of decaying discrepancy data using regression with absolute tolerances
- short polynomialOrder

  scalar integer indicating the order of the polynomial approximation (1=linear, 2=quadratic, 3=cubic; from the `polynomial` *specification in ModelSurrG)*
- RealVector krigingCorrelations

  vector of correlations used in building a kriging approximation (from the `correlations` *specification in ModelSurrG)*
- String krigingOptMethod

  optimization method to use in finding optimal correlation parameters: none, sampling, local, global
- short krigingMaxTrials

maximum number of trials in optimization of kriging correlations

- RealVector krigingMaxCorrelations

  upper bound on kriging correlation vector

- RealVector krigingMinCorrelations

  lower bound on kriging correlation vector

- Real krigingNugget

  nugget value for kriging

- short krigingFindNugget

  option to have Kriging find the best nugget value to use

- short mlsWeightFunction

  weight function for moving least squares approximation

- short rbfBases

  bases for radial basis function approximation

- short rbfMaxPts

  maximum number of points for radial basis function approximation

- short rbfMaxSubsets

  maximum number of subsets for radial basis function approximation

- short rbfMinPartition

  minimum partition for radial basis function approximation

- short marsMaxBases

  maximum number of bases for MARS approximation

- String marsInterpolation

  interpolation type for MARS approximation

- short annRandomWeight

  random weight for artificial neural network approximation

- short annNodes

  number of nodes for artificial neural network approximation

- Real annRange

  range for artificial neural network approximation

- int numRestarts

  number of restarts for gradient-based optimization in GP

- bool domainDecomp

  whether domain decomposition is enabled

- String decompCellType

  type of local cell of domain decomp

- int decompSupportLayers

  number of support layers for each local basis function

- bool decompDiscontDetect

  whether discontinuity detection is enabled

- Real discontJumpThresh

  function value (jump) threshold for discontinuity detection in domain decomp

- Real discontGradThresh

  gradient threshold for discontinuity detection in domain decomp

- String trendOrder

  scalar integer indicating the order of the Gaussian process mean (0= constant, 1=linear, 2=quadratic, 3=cubic); from the `gaussian_process` specification in ModelSurrG)

- bool pointSelection

  flag indicating the use of point selection in the Gaussian process

- StringArray diagMetrics

  List of diagnostic metrics the user requests to assess the goodness of fit for a surrogate model.

- bool crossValidateFlag

flag indicating the use of cross validation on the metrics specified

- int numFolds

  number of folds to perform in cross validation

- Real percentFold

  percentage of data to withhold for cross validation process

- bool pressFlag

  flag indicating the use of PRESS on the metrics specified

- String importChallengePtsFile

  the file name from the `challenge_points_file` specification in ModelSurrG

- unsigned short importChallengeFormat

  tabular format of the challenge data file

- bool importChalUseVariableLabels

  whether to parse/validate variable labels from header

- bool importChallengeActive

  whether to import active variables only

- String advancedOptionsFilename

  file containing advanced surrogate option overrides

- String optionalInterfRespPointer

  string pointer to the responses specification used by the optional interface in nested models (from the `optional-_interface_responses_pointer` specification in ModelNested)

- StringArray primaryVarMaps

  the primary variable mappings used in nested models for identifying the lower level variable targets for inserting top level variable values (from the `primary_variable_mapping` specification in ModelNested)

- StringArray secondaryVarMaps

  the secondary variable mappings used in nested models for identifying the (distribution) parameter targets within the lower level variables for inserting top level variable values (from the `secondary_variable_mapping` specification in ModelNested)

- RealVector primaryRespCoeffs

  the primary response mapping matrix used in nested models for weighting contributions from the sub-iterator responses in the top level (objective) functions (from the `primary_response_mapping` specification in ModelNested)

- RealVector secondaryRespCoeffs

  the secondary response mapping matrix used in nested models for weighting contributions from the sub-iterator responses in the top level (constraint) functions (from the `secondary_response_mapping` specification in ModelNested)

- bool identityRespMap

  whether an identity response map is requested in lieu of explicit maps

- int subMethodServers

  number of servers for concurrent sub-iterator parallelism

- int subMethodProcs

  number of processors for each concurrent sub-iterator partition

- short subMethodScheduling

  scheduling approach for concurrent sub-iterator parallelism: {DEFAULT,MASTER,PEER}_SCHEDULING

- int initialSamples

  initial samples to build the subspace model

- unsigned short subspaceSampleType

  sampling method for building the subspace model

- IntVector refineSamples

  refinement samples to add in each batch

- size_t maxIterations

  maximum number of subspace build iterations

- Real convergenceTolerance

convergence tolerance on build process
- bool subspaceIdBingLi

  Flag to use Bing Li method to identify active subspace dimension.
- bool subspaceIdConstantine

  Flag to use Constantine method to identify active subspace dimension.
- bool subspaceIdEnergy

  Flag to use eigenvalue energy method to identify active subspace dimension.
- bool subspaceBuildSurrogate

  Flag to build surrogate over active subspace.
- int subspaceDimension

  Size of subspace.
- unsigned short subspaceNormalization

  Normalization to use when forming a subspace with multiple response functions.
- int numReplicates

  Number of bootstrap samples for subspace identification.
- bool subspaceIdCV

  Flag to use cross validation to identify active subspace dimension.
- Real relTolerance

  relative tolerance used by cross validation subspace dimension id method
- Real decreaseTolerance

  decrease tolerance used by cross validation subspace dimension id method
- int subspaceCVMaxRank

  maximum rank considered by cross validation subspace dimension id method
- bool subspaceCVIncremental

  flag to use incremental dimension estimation in the cross validation metric
- unsigned short subspaceIdCVMethod

  Contains which cutoff method to use in the cross validation metric.
- short regressionType

  type of (regularized) regression: FT_LS or FT_RLS2
- Real regressionL2Penalty

  penalty parameter for regularized regression (FT_RLS2)
- size_t maxSolverIterations

  max iterations for optimization solver used in FT regression
- int maxCrossIterations

  maximum number of cross iterations
- Real solverTol

  optimization tolerance for FT regression
- Real solverRoundingTol

  Rounding tolerance for FT regression.
- Real statsRoundingTol

  arithmetic (rounding) tolerance for FT sums and products
- bool tensorGridFlag

  sub-sample a tensor grid for generating regression data
- unsigned short startOrder

  starting polynomial order
- unsigned short kickOrder

  polynomial order increment when adapting
- unsigned short maxOrder

  maximum order of basis polynomials
- bool adaptOrder

  whether or not to adapt order by cross validation

- size_t startRank

  starting rank
- size_t kickRank

  rank increase increment
- size_t maxRank

  maximum rank
- bool adaptRank

  whether or not to adapt rank
- size_t maxCVRankCandidates

  maximum number of cross-validation candidates for adaptRank
- unsigned short maxCVOrderCandidates

  maximum number of cross-validation candidates for adaptOrder
- short c3AdvanceType

  quantity to increment (start rank, start order, max rank, max order, max rank + max order) for FT (uniform) p-refinement
- size_t collocationPoints

  number of data points used in FT construction by regression
- Real collocationRatio

  ratio of number of points to nuber of unknowns
- bool autoRefine

  whether automatic surrogate refinement is enabled
- size_t maxFunctionEvals

  maximum evals in refinement
- String refineCVMetric

  metric to use in cross-validation guided refinement
- int softConvergenceLimit

  max number of iterations in refinement without improvement
- int refineCVFolds

  number of cross-validation folds in guided refinement
- unsigned short adaptedBasisSparseGridLev

  sparse grid level for low-order PCE used to compute rotation matrix within adapted basis approach to dimension reduction
- unsigned short adaptedBasisExpOrder

  expansion order for low-order PCE used to compute rotation matrix within adapted basis approach to dimension reduction
- Real adaptedBasisCollocRatio

  collocation ratio for low-order PCE used to compute rotation matrix within adapted basis approach to dimension reduction
- short **method_rotation**
- Real **adaptedBasisTruncationTolerance**
- unsigned short randomFieldIdForm

  Contains which type of random field model.
- unsigned short analyticCovIdForm

  Contains which type of analytic covariance function.
- Real truncationTolerance

  truncation tolerance on build process: percent variance explained
- String propagationModelPointer

  pointer to the model through which to propagate the random field
- String rfDataFileName

  File from which to build the random field.

Private Member Functions

- DataModelRep ()

    constructor
- void write (std::ostream &s) const

    write a DataModelRep object to an std::ostream
- void read (MPIUnpackBuffer &s)

    read a DataModelRep object from a packed MPI buffer
- void write (MPIPackBuffer &s) const

    write a DataModelRep object to a packed MPI buffer

Friends

- class DataModel

    the handle class can access attributes of the body class directly

14.52.1 Detailed Description

Body class for model specification data.

The DataModelRep class is used to contain the data from a model keyword specification. Default values are managed in the DataModelRep constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::dataModelList is private.

The documentation for this class was generated from the following files:

- DataModel.hpp
- DataModel.cpp

14.53 DataResponses Class Reference

Handle class for responses specification data.

Public Member Functions

- DataResponses ()

    constructor
- DataResponses (const DataResponses &)

    copy constructor
- ∼DataResponses ()

    destructor
- DataResponses & operator= (const DataResponses &)

    assignment operator
- void write (std::ostream &s) const

    write a DataResponses object to an std::ostream
- void read (MPIUnpackBuffer &s)

    read a DataResponses object from a packed MPI buffer
- void write (MPIPackBuffer &s) const

    write a DataResponses object to a packed MPI buffer
- std::shared_ptr< DataResponsesRep > data_rep ()

    return dataRespRep

Static Public Member Functions

- static bool id_compare (const DataResponses &dr, const std::string &id)

  compares the idResponses attribute of DataResponses objects

Private Attributes

- std::shared_ptr< DataResponsesRep > dataRespRep

  pointer to the body (handle-body idiom)

Friends

- class **ProblemDescDB**
- class **NIDRProblemDescDB**

14.53.1 Detailed Description

Handle class for responses specification data.

The DataResponses class is used to provide a memory management handle for the data in DataResponsesRep. It is populated by IDRProblemDescDB::responses_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataResponses objects is maintained in ProblemDescDB::dataResponsesList, one for each responses specification in an input file.

The documentation for this class was generated from the following files:

- DataResponses.hpp
- DataResponses.cpp

14.54 DataResponsesRep Class Reference

Body class for responses specification data.

Public Member Functions

- ∼DataResponsesRep ()

  destructor

Public Attributes

- String idResponses

  string identifier for the responses specification data set (from the `id_responses` specification in RespSetId)
- StringArray responseLabels

  the response labels array (from the `response_descriptors` specification in RespLabels)
- size_t numObjectiveFunctions

  number of objective functions (from the `num_objective_functions` specification in RespFnOpt)
- size_t numLeastSqTerms

  number of least squares terms (from the `num_calibration_terms` specification in RespFnLS)
- size_t numNonlinearIneqConstraints

  number of nonlinear inequality constraints (from the `num_nonlinear_inequality_constraints` specification in RespFnOpt)

- size_t numNonlinearEqConstraints

  number of nonlinear equality constraints (from the `num_nonlinear_equality_constraints` *specification in RespFnOpt)*
- size_t numResponseFunctions

  number of generic response functions (from the `num_response_functions` *specification in RespFnGen)*
- size_t numScalarObjectiveFunctions

  scalar_objectives: number of objective functions which are scalar
- size_t numScalarLeastSqTerms

  scalar_calibration_terms: number of calibration terms which are scalar
- size_t numScalarNonlinearIneqConstraints

  number of scalar nonlinear inequality constraints (from the `num_scalar_nonlinear_inequality_constraints` *specification in RespFnOpt)*
- size_t numScalarNonlinearEqConstraints

  number of scalar nonlinear equality constraints (from the `num_scalar_nonlinear_equality_constraints` *specification in RespFnOpt)*
- size_t numScalarResponseFunctions

  scalar_responses: number of response functions which are scalar
- size_t numFieldObjectiveFunctions

  field_objectives: number of objective functions which are field-valued
- size_t numFieldLeastSqTerms

  field_calibration_terms: number of calibration terms which are field-valued
- size_t numFieldNonlinearIneqConstraints

  number of field nonlinear inequality constraints (from the `num_scalar_nonlinear_inequality_constraints` *specification in RespFnOpt)*
- size_t numFieldNonlinearEqConstraints

  number of field nonlinear equality constraints (from the `num_scalar_nonlinear_equality_constraints` *specification in RespFnOpt)*
- size_t numFieldResponseFunctions

  field_responses: number of response functions which are field-valued
- StringArray primaryRespFnSense

  optimization sense for each objective function: minimize or maximize
- RealVector primaryRespFnWeights

  vector of weightings for multiobjective optimization or weighted nonlinear least squares (from the `multi_objective_weights` *specification in RespFnOpt and the* `least_squares_weights` *specification in RespFnLS)*
- RealVector nonlinearIneqLowerBnds

  vector of nonlinear inequality constraint lower bounds (from the `nonlinear_inequality_lower_bounds` *specification in RespFnOpt)*
- RealVector nonlinearIneqUpperBnds

  vector of nonlinear inequality constraint upper bounds (from the `nonlinear_inequality_upper_bounds` *specification in RespFnOpt)*
- RealVector nonlinearEqTargets

  vector of nonlinear equality constraint targets (from the `nonlinear_equality_targets` *specification in RespFnOpt)*
- StringArray primaryRespFnScaleTypes

  vector of primary response function scaling types (from the `objective_function_scale_types` *specification in RespFnOpt and the* `least_squares_term_scale_types` *specification in RespFnLS)*
- RealVector primaryRespFnScales

  vector of primary response function scaling factors (from the `objective_function_scales` *specification in RespFnOpt and the* `least_squares_term_scales` *specification in RespFnLS)*
- StringArray nonlinearIneqScaleTypes

  vector of nonlinear inequality constraint scaling types (from the `nonlinear_inequality_scale_types` *specification in RespFnOpt)*

- RealVector nonlinearIneqScales

    vector of nonlinear inequality constraint scaling factors (from the `nonlinear_inequality_scales` *specification in RespFnOpt)*
- StringArray nonlinearEqScaleTypes

    vector of nonlinear equality constraint scaling types (from the `nonlinear_equality_scale_types` *specification in RespFnOpt)*
- RealVector nonlinearEqScales

    vector of nonlinear equality constraint scaling factors (from the `nonlinear_equality_scales` *specification in RespFnOpt)*
- bool calibrationDataFlag

    whether calibration data was specified
- size_t numExperiments

    number of distinct experiments in experimental data
- size_t numExpConfigVars

    number of experimental configuration vars (state variables) in each row of data
- RealVector expConfigVars

    list of num_experiments x num_config_vars configuration variable values
- RealVector simVariance

    list of variances of errors to be added to simulation responses
- bool interpolateFlag

    whether one should interpolate between the experiment and simulation field data
- RealVector expObservations

    list of num_calibration_terms observation data
- RealVector expStdDeviations

    list of 1 or num_calibration_terms observation standard deviations
- String scalarDataFileName

    name of experimental data file containing response data (with optional state variable and sigma data) to read
- unsigned short scalarDataFormat

    tabular format of the scalar data file
- String gradientType

    gradient type: none, numerical, analytic, or mixed (from the `no_gradients`, `numerical_gradients`, `analytic_gradients`, *and* `mixed_gradients` *specifications in RespGrad)*
- String hessianType

    Hessian type: none, numerical, quasi, analytic, or mixed (from the `no_hessians`, `numerical_hessians`, `quasi_hessians`, `analytic_hessians`, *and* `mixed_hessians` *specifications in RespHess)*
- bool ignoreBounds

    option to ignore bounds when doing finite differences (default is to honor bounds)
- bool centralHess

    Temporary(?) option to use old 2nd-order diffs when computing finite-difference Hessians; default is forward differences.
- String quasiHessianType

    quasi-Hessian type: bfgs, damped_bfgs, or sr1 (from the `bfgs` *and* `sr1` *specifications in RespHess)*
- String methodSource

    numerical gradient method source: dakota or vendor (from the `method_source` *specification in RespGradNum and RespGradMixed)*
- String intervalType

    numerical gradient interval type: forward or central (from the `interval_type` *specification in RespGradNum and RespGradMixed)*
- RealVector fdGradStepSize

    vector of finite difference step sizes for numerical gradients, one step size per active continuous variable, used in computing 1st-order forward or central differences (from the `fd_gradient_step_size` *specification in RespGradNum and RespGradMixed)*
- String fdGradStepType

type of finite difference step to use for numerical gradient: relative - step length is relative to x absolute - step length is what is specified bounds - step length is relative to range of x

- RealVector fdHessStepSize

  vector of finite difference step sizes for numerical Hessians, one step size per active continuous variable, used in computing 1st-order gradient-based differences and 2nd-order function-based differences (from the `fd_hessian_step_size` specification in RespHessNum and RespHessMixed)

- String fdHessStepType

  type of finite difference step to use for numerical Hessian: relative - step length is relative to x absolute - step length is what is specified bounds - step length is relative to range of x

- IntSet idNumericalGrads

  mixed gradient numerical identifiers (from the `id_numerical_gradients` specification in RespGradMixed)

- IntSet idAnalyticGrads

  mixed gradient analytic identifiers (from the `id_analytic_gradients` specification in RespGradMixed)

- IntSet idNumericalHessians

  mixed Hessian numerical identifiers (from the `id_numerical_hessians` specification in RespHessMixed)

- IntSet idQuasiHessians

  mixed Hessian quasi identifiers (from the `id_quasi_hessians` specification in RespHessMixed)

- IntSet idAnalyticHessians

  mixed Hessian analytic identifiers (from the `id_analytic_hessians` specification in RespHessMixed)

- String dataPathPrefix

  path to prepend to any data file names

- IntVector fieldLengths

  number of entries in each field

- IntVector numCoordsPerField

  number of coordinates per field

- bool readFieldCoords

  Field data related storage: whether to read simulation field coordinates.

- StringArray varianceType

  `Array which specifies the sigma type per response (none, one`
  constant value, one per response (vector) or a full covariance matrix

- StringArray metadataLabels

  descriptors for each metadata field

Private Member Functions

- DataResponsesRep ()

  constructor

- void write (std::ostream &s) const

  write a DataResponsesRep object to an std::ostream

- void read (MPIUnpackBuffer &s)

  read a DataResponsesRep object from a packed MPI buffer

- void write (MPIPackBuffer &s) const

  write a DataResponsesRep object to a packed MPI buffer

Friends

- class DataResponses

  the handle class can access attributes of the body class directly

14.54.1 Detailed Description

Body class for responses specification data.

The DataResponsesRep class is used to contain the data from a responses keyword specification. Default values are managed in the DataResponsesRep constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::dataResponsesList is private.

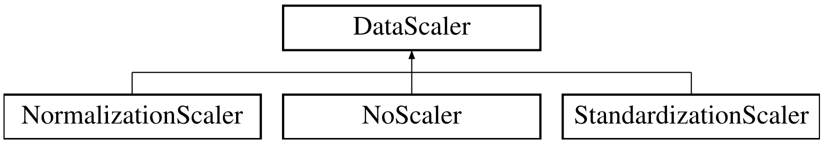
The documentation for this class was generated from the following files:

- DataResponses.hpp
- DataResponses.cpp

14.55 DataScaler Class Reference

The DataScaler class computes the scaling coefficients and scales a 2D data matrix with dimensions num_samples by num_features.

Inheritance diagram for DataScaler:



Public Types

- enum SCALER_TYPE { **NONE**, **STANDARDIZATION**, **MEAN_NORMALIZATION**, **MINMAX_NORMALIZATION** }

  Enumeration for supported types of DataScalers.

Public Member Functions

- void scale_samples (const MatrixXd &unscaled_samples, MatrixXd &scaled_samples)

  Apply scaling to a set of unscaled samples.
- MatrixXd scale_samples (const MatrixXd &unscaled_samples)

  Apply scaling to a set of unscaled samples.
- const VectorXd & get_scaler_features_offsets () const

  Get the vector of offsets.
- const VectorXd & get_scaler_features_scale_factors () const

  Get the vector of scaling factors.
- bool check_for_zero_scaler_factor (int index)

  Checks an individual scaler feature scale factor for being close to zero; If it is near zero, we can potentially run into a divide-by-zero error if not handled appropriately.

Static Public Member Functions

- static SCALER_TYPE scaler_type (const std::string &scaler_name)

  Convert scaler name to enum type.

Protected Attributes

- bool hasScaling

    Bool for whether or not the the scaling coefficients have been computed.
- RowVectorXd scaledSample

    Vector for a single scaled sample - (num_features); avoids resize memory allocs.
- VectorXd scalerFeaturesOffsets

    Vector of offsets - (num_features)
- VectorXd scalerFeaturesScaleFactors

    Vector of scaling factors - (num_features)

Private Member Functions

- template<class Archive >
  void serialize (Archive &archive, const unsigned int version)

    Serializer for base class data (call from dervied with base_object)

Friends

- class boost::serialization::access

    Allow serializers access to private class data.

14.55.1 Detailed Description

The DataScaler class computes the scaling coefficients and scales a 2D data matrix with dimensions num_samples by num_features.

There are currently 3 scaling options for the DataScaler class:

1. StandardizationScaler - transform each feature to have zero mean and unit variance.
2. NormalizationScaler - normalizies each feature uses the max and min value divided by either the mean value (mean_normalization = true) or min value (mean_normalization = false) Also allows for a norm_factor scaling, required for the direct neural network.
3. NoScaler - scaling coefficients amount to an identity operation

14.55.2 Member Function Documentation

14.55.2.1 void scale_samples (const MatrixXd & *unscaled_samples*, MatrixXd & *scaled_samples*)

Apply scaling to a set of unscaled samples.

Parameters

in	*unscaled_-samples*	Unscaled matrix of samples
out	*scaled_samples*	Scaled matrix of samples

References DataScaler::check_for_zero_scaler_factor(), DataScaler::scalerFeaturesOffsets, and DataScaler::scalerFeaturesScaleFactors.

Referenced by PolynomialRegression::build(), GaussianProcess::build(), GaussianProcess::covariance(), PolynomialRegression::gradient(), GaussianProcess::gradient(), PolynomialRegression::hessian(), GaussianProcess::hessian(), DataScaler::scale_samples(), PolynomialRegression::value(), and GaussianProcess::value().

14.55.2.2 MatrixXd scale_samples (const MatrixXd & *unscaled_samples*) [inline]

Apply scaling to a set of unscaled samples.

Parameters

in	*unscaled_-samples*	Unscaled matrix of samples

Returns

MatrixXd scaled_samples Scaled matrix of samples

References DataScaler::scale_samples().

14.55.2.3 const VectorXd& get_scaler_features_offsets ( ) const [inline]

Get the vector of offsets.

Returns

Vector of scaler offsets - (num_features)

References DataScaler::scalerFeaturesOffsets.

14.55.2.4 const VectorXd& get_scaler_features_scale_factors ( ) const [inline]

Get the vector of scaling factors.

Returns

Vector of scaling factors - (num_features)

References DataScaler::scalerFeaturesScaleFactors.

Referenced by dakota::surrogates::fd_check_gradient(), and dakota::surrogates::fd_check_hessian().

14.55.2.5 bool check_for_zero_scaler_factor (int *index*)

Checks an individual scaler feature scale factor for being close to zero; If it is near zero, we can potentially run into a divide-by-zero error if not handled appropriately.

Parameters

in	*index*	The scaler feature index to check

Returns

True if the value is near zero

References dakota::near_zero, and DataScaler::scalerFeaturesScaleFactors.

Referenced by DataScaler::scale_samples().

14.55.2.6 SCALER_TYPE scaler_type (const std::string & *scaler_name*) [static]

Convert scaler name to enum type.

Parameters

in	*scaler_name*	DataScaler name to map

Returns

Corresponding DataScaler enum

References dakota::util::type_name_bimap.

Referenced by PolynomialRegression::build(), and GaussianProcess::build().

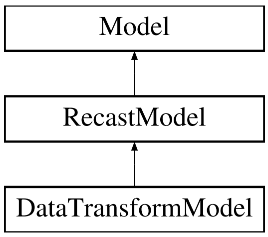
The documentation for this class was generated from the following files:

- UtilDataScaler.hpp
- UtilDataScaler.cpp

14.56 DataTransformModel Class Reference

Data transformation specialization of RecastModel.

Inheritance diagram for DataTransformModel:



Public Member Functions

- DataTransformModel (const Model &sub_model, const ExperimentData &exp_data, size_t num_hyper=0, unsigned short mult_mode=CALIBRATE_NONE, short recast_resp_deriv_order=1)

    standard constructor
- ∼DataTransformModel ()

    destructor
- void data_transform_response (const Variables &sub_model_vars, const Response &sub_model_resp, Response &residual_resp)

    Convenience function to help recover a residual response from the submodel.
- void data_resize ()

    The size of the ExperimentData changed; update the residualModel size.
- void print_best_responses (std::ostream &s, const Variables &best_submodel_vars, const Response &best_submodel_resp, size_t num_best, size_t best_ind)

    manage best responses including residuals and model responses per config
- void archive_best_responses (const ResultsManager &results_db, const StrStrSizet iterator_id, const Variables &best_submodel_vars, const Response &best_submodel_resp, size_t num_best, size_t best_ind)

    archive best responses
- int num_config_vars () const

    return number of configuration variables

Protected Types

- typedef std::map< int, IntResponseMap > **IntIntResponseMapMap**

Protected Member Functions

- void assign_instance ()

  assign static pointer instance to this for use in static transformation functions
- void init_metadata () override

  default clear metadata in Recasts; derived classes can override to no-op
- void update_from_subordinate_model (size_t depth=SZ_MAX)

  propagate vars/labels/bounds/targets from the bottom up
- void update_cv_skip_hyperparams (const Model &model)

  update all continuous variables from sub-model, skipping hyper-parameters
- void expand_linear_constraints (const Model &model)

  expand linear constraints from sub-model to account for hyper-parameters
- void update_expanded_response (const Model &model)

  update currentResponse based on replicate experiment data
- void gen_primary_resp_map (const SharedResponseData &srd, Sizet2DArray &primary_resp_map_indices, BoolDequeArray &nonlinear_resp_map) const

  compute the primary response map for a data transform RecastModel
- void derived_evaluate (const ActiveSet &set)

  specialization of evaluate that iterates over configuration variables
- void derived_evaluate_nowait (const ActiveSet &set)

  specialization of evaluate that iterates over configuration variables
- const IntResponseMap & derived_synchronize ()

  synchronize all evaluations (all residuals for all experiment configurations)
- const IntResponseMap & derived_synchronize_nowait ()

  return any evaluations for which all experiment configurations have completed
- const IntResponseMap & filter_submodel_responses ()
- void cache_submodel_responses (const IntResponseMap &sm_resp_map, bool deep_copy)

  cache the subModel responses into a per-RecastModel eval ID map
- void collect_residuals (bool collect_all)

  collect any (or force all) completed subModel evals and populate recastResponseMap with residuals for those that are fully completed
- void transform_response_map (const IntResponseMap &submodel_resp, const Variables &recast_vars, Response &residual_resp)

  transform a set of per-configuration subModel Responses to a single evaluation's residuals
- void scale_response (const Variables &submodel_vars, const Variables &recast_vars, Response &recast_response)

  scale the populated residual response by any covariance information, including hyper-parameter multipliers
- void init_continuous_vars ()

  Initialize continuous variable values/labels.
- template<typename T >
  void expand_primary_array (size_t submodel_size, const T &submodel_array, size_t recast_size, T &recast_array) const

  (if non-empty) expand submodel_array by replicates to populate a recast_array
- void **print_residual_response** (const Response &resid_resp)
- void **recover_submodel_responses** (std::ostream &s, const Variables &best_submodel_vars, size_t num_best, size_t best_ind, Response &residual_resp)

- void archive_submodel_responses (const ResultsManager &results_db, const StrStrSizet &iterator_id, const Variables &best_submodel_vars, size_t num_best, size_t best_ind, Response &residual_resp)

    archive original model responses

- void archive_best_original (const ResultsManager &results_db, const StrStrSizet &iterator_id, const RealVector &function_values, const int &exp_index, const int &num_best, const int &best_index)

    Archive the best model reponses (undifferenced with experimental data) for experiment exp_index and final solution soln_index.

- void archive_best_config_variables (const ResultsManager &results_db, const StrStrSizet &iterator_id, const Variables &vars, const int &exp_index, const int &num_best, const int &best_index)

    Archive the best configuration variables associated with each model response.

- void archive_best_residuals (const ResultsManager &results_db, const StrStrSizet &iterator_id, const int num_fns, const RealVector &best_terms, const Real wssr, const int num_points, const int point_index)

    Archive the best residuals.

Static Protected Member Functions

- static SizetArray variables_expand (const Model &sub_model, size_t num_hyper)

    expand the variable counts to account for hyper-parameters

- static int get_hyperparam_vc_index (const Model &sub_model)

    determine the index into vc_totals corresponding to where the hyper-parameters go

- static short response_order (const Model &sub_model, short recast_resp_order=1)

    helper to compute the recast response order during member initialization; recast_resp_order passed is the minimum request client needs

- static void vars_mapping (const Variables &recast_vars, Variables &submodel_vars)

    map the inbound expanded variables to the sub-model, discarding hyperparams (assumes hyper-parameters are at end of active continuous variables)

- static void set_mapping (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)

    map the inbound ActiveSet to the sub-model (map derivative variables)

- static void primary_resp_differencer (const Variables &submodel_vars, const Variables &recast_vars, const Response &submodel_response, Response &recast_response)

    Recast callback function to difference residuals with observed data.

Protected Attributes

- const ExperimentData & expData

    Reference to the experiment data used to construct this Model.

- size_t numHyperparams

    Number of calibrated variance multipliers.

- unsigned short obsErrorMultiplierMode

    Calibration mode for the hyper-parameters.

- IntIntResponseMapMap **cachedResp**

Static Protected Attributes

- static DataTransformModel $*$ dtModelInstance

    static pointer to this class for use in static callbacks

Additional Inherited Members

14.56.1 Detailed Description

Data transformation specialization of RecastModel.

Specialization of RecastModel to create a residual model that maps (1) from an augmented set of calibration parameters (including hyper-parameters) to those needed by the underlying simulation model and (2) from the simulation model response to a set of residuals, whose overall size may differ from the simulation (sub-model) response. The residuals may be scaled by experiment covariance information. This class provides a simple constructor that forwards to the more complicated RecastModel API

14.56.2 Constructor & Destructor Documentation

14.56.2.1 DataTransformModel (const Model & *sub_model*, const ExperimentData & *exp_data*, size_t *num_hyper* = 0, unsigned short *mult_mode* = CALIBRATE_NONE, short *recast_resp_deriv_order* = 1)

standard constructor

This constructor computes various indices and mappings, then updates the properties of the RecastModel. Hyper-parameters are assumed to trail the active continuous variables when presented to this RecastModel

References Dakota::abort_handler(), Model::current_response(), Model::cv(), Model::div(), Model::drv(), Model::dsv(), DataTransformModel::expData, DataTransformModel::gen_primary_resp_map(), Model::icv(), Model::idiv(), Model::idrv(), Model::idsv(), Model::inactive_view(), DataTransformModel::init_continuous_vars(), RecastModel::init_maps(), Model::modelId, Model::multivariate_distribution(), Model::mvDist, DataTransformModel::num_config_vars(), ExperimentData::num_config_vars(), Model::num_primary_fns(), Model::num_secondary_fns(), ExperimentData::num_total_exppoints(), DataTransformModel::numHyperparams, DataTransformModel::primary_resp_differencer(), RecastModel::recast_model_id(), RecastModel::root_model_id(), DataTransformModel::set_mapping(), Response::shared_data(), RecastModel::subModel, DataTransformModel::update_expanded_response(), and DataTransformModel::vars_mapping().

14.56.3 Member Function Documentation

14.56.3.1 void update_from_subordinate_model (size_t *depth* = SZ_MAX) [protected], [virtual]

propagate vars/labels/bounds/targets from the bottom up

used only for instantiate-on-the-fly model recursions (all RecastModel instantiations and alternate DataFitSurrModel instantiations). Simulation, Hierarchical, and Nested Models do not redefine the function since they do not support instantiate-on-the-fly. This means that the recursion will stop as soon as it encounters a Model that was instantiated normally, which is appropriate since ProblemDescDB-constructed Models use top-down information flow and do not require bottom-up updating.

Reimplemented from Model.

References DataTransformModel::expand_linear_constraints(), Model::multivariate_distribution(), Model::mvDist, DataTransformModel::numHyperparams, RecastModel::subModel, Dakota::SZ_MAX, DataTransformModel::update_cv_skip_hyperparams(), RecastModel::update_discrete_variable_bounds(), RecastModel::update_discrete_variable_labels(), RecastModel::update_discrete_variable_values(), DataTransformModel::update_expanded_response(), Model::update_from_subordinate_model(), RecastModel::update_variables_active_complement_from_model(), and RecastModel::update_variables_from_model().

14.56.3.2 void update_expanded_response (const Model & *model*) [protected]

update currentResponse based on replicate experiment data

Expand response-related arrays, accounting for multiple experiments and/or interpolation.

References Model::currentResponse, DataTransformModel::expand_primary_array(), DataTransformModel::expData, ExperimentData::fill_primary_function_labels(), SharedResponseData::function_labels(), ExperimentData::interpolate_flag(), Model::num_primary_fns(), ExperimentData::num_total_exppoints(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), Model::primaryRespFnSense, Model::primaryRespFnWts, ScalingOptions::priScales, ScalingOptions::priScaleTypes, Model::scaling_options(), Model::scalingOpts, Response::shared_data(), and RecastModel::update_secondary_response().

Referenced by DataTransformModel::DataTransformModel(), and DataTransformModel::update_from_subordinate_model().

14.56.3.3 SizetArray variables_expand (const Model & *sub_model*, size_t *num_hyper*) [static], [protected]

expand the variable counts to account for hyper-parameters

Incorporate the hyper parameters into Variables, assuming they are at the end of the active continuous variables. For example, append them to continuous design or continuous aleatory uncertain.

References SharedVariablesData::components_totals(), Model::current_variables(), DataTransformModel::get_hyperparam_vc_index(), Variables::shared_data(), and Dakota::svd().

14.56.3.4 void derived_evaluate (const ActiveSet & *set*) [protected], [virtual]

specialization of evaluate that iterates over configuration variables

Blocking evaluation over all experiment configurations to compute a single set of expanded residuals. If the subModel supports asynchronous evaluate_nowait(), do the configuration evals concurrently and then synchronize.

Reimplemented from Model.

References Response::active_set(), Model::asynch_flag(), Model::current_response(), Model::current_variables(), Model::currentResponse, Model::currentVariables, RecastModel::derived_evaluate(), Model::evaluate(), Model::evaluate_nowait(), Model::evaluation_id(), DataTransformModel::expData, DataTransformModel::filter_submodel_responses(), ExperimentData::form_residuals(), Model::inactive_variables(), ExperimentData::num_config_vars(), ExperimentData::num_experiments(), Model::outputLevel, RecastModel::recastIdMap, RecastModel::recastModelEvalCntr, DataTransformModel::scale_response(), RecastModel::subModel, DataTransformModel::transform_response_map(), RecastModel::transform_set(), and RecastModel::transform_variables().

14.56.3.5 void derived_evaluate_nowait (const ActiveSet & *set*) [protected], [virtual]

specialization of evaluate that iterates over configuration variables

Non-blocking evaluation (scheduling) over all experiment configurations. Assumes that if this model supports nowait, its subModel does too and schedules them all.

Reimplemented from Model.

References Variables::copy(), Model::current_variables(), Model::currentVariables, RecastModel::derived_evaluate_nowait(), Model::evaluate_nowait(), Model::evaluation_id(), DataTransformModel::expData, Model::inactive_variables(), ExperimentData::num_config_vars(), ExperimentData::num_experiments(), Model::outputLevel, RecastModel::recastIdMap, RecastModel::recastModelEvalCntr, RecastModel::recastSetMap, RecastModel::recastVarsMap, RecastModel::subModel, RecastModel::transform_set(), and RecastModel::transform_variables().

14.56.3.6 const IntResponseMap & derived_synchronize ( ) [protected], [virtual]

synchronize all evaluations (all residuals for all experiment configurations)

Collect all the subModel evals and build the residual sets for all evaluations. Like rekey functions in DakotaModel, but many sub-model to one recast-model. For the blocking synchronize case, we force the subModel to synch and have all needed data.

Reimplemented from Model.

References DataTransformModel::cache_submodel_responses(), DataTransformModel::collect_residuals(), RecastModel::derived_synchronize(), DataTransformModel::expData, ExperimentData::num_config_vars(), RecastModel::recastResponseMap, RecastModel::subModel, and Model::synchronize().

14.56.3.7 const IntResponseMap & derived_synchronize_nowait ( ) [protected], [virtual]

return any evaluations for which all experiment configurations have completed

Collect any completed subModel evals and build the residual sets for any fully completed evaluations. Like rekey functions in DakotaModel, but many sub-model to one recast-model. We do not force the subModel to synch.

Reimplemented from Model.

References DataTransformModel::cache_submodel_responses(), DataTransformModel::collect_residuals(), RecastModel::derived_synchronize_nowait(), DataTransformModel::expData, ExperimentData::num_config_vars(), RecastModel::recastResponseMap, RecastModel::subModel, and Model::synchronize_nowait().

14.56.3.8 const IntResponseMap & filter_submodel_responses ( ) [protected]

(We don't quite want the rekey behavior since multiple subModel evals map to one recast eval.)

References Model::cache_unmatched_response(), RecastModel::recastIdMap, RecastModel::subModel, and Model::synchronize().

Referenced by DataTransformModel::derived_evaluate().

14.56.3.9 void transform_response_map (const IntResponseMap & *submodel_resp*, const Variables & *recast_vars*, Response & *residual_resp*) [protected]

transform a set of per-configuration subModel Responses to a single evaluation's residuals

This transformation assumes the residuals are in submodel eval_id order.

References Dakota::abort_handler(), Model::current_variables(), DataTransformModel::expData, ExperimentData::form_residuals(), ExperimentData::num_experiments(), DataTransformModel::scale_response(), and RecastModel::subModel.

Referenced by DataTransformModel::collect_residuals(), and DataTransformModel::derived_evaluate().

14.56.3.10 void set_mapping (const Variables & *recast_vars*, const ActiveSet & *recast_set*, ActiveSet & *sub_model_set*) [static], [protected]

map the inbound ActiveSet to the sub-model (map derivative variables)

RecastModel sets up a default set mapping before calling this update, so focus on updating the derivative variables vector

References Model::cv(), ActiveSet::derivative_vector(), DataTransformModel::dtModelInstance, DataTransformModel::numHyperparams, ActiveSet::request_vector(), and RecastModel::subordinate_model().

Referenced by DataTransformModel::DataTransformModel().

14.56.3.11 void init_continuous_vars ( ) [protected]

Initialize continuous variable values/labels.

Pull up the continuous variable values and labels into the RecastModel, inserting the hyper-parameter values/labels

References Model::all_continuous_lower_bound(), Model::all_continuous_lower_bounds(), Model::all_continuous_upper_bound(), Model::all_continuous_upper_bounds(), Model::all_continuous_variable(), Model::all_continuous_variable_label(), Model::all_continuous_variable_labels(), Model::all_continuous_variables(), SharedVariables-

Data::components_totals(), Model::current_variables(), DataTransformModel::expData, DataTransformModel::get_hyperparam_vc_index(), ExperimentData::hyperparam_labels(), DataTransformModel::numHyperparams, DataTransformModel::obsErrorMultiplierMode, Variables::shared_data(), RecastModel::subModel, and Dakota::svd().

Referenced by DataTransformModel::DataTransformModel().

14.56.3.12 void expand_primary_array (size_t *submodel_size,* const T & *submodel_array,* size_t *recast_size,* T & *recast_array*) const [protected]

(if non-empty) expand submodel_array by replicates to populate a recast_array

If size greater than 1, expand submodel_array by replicates to populate a pre-sized recast_array, otherwise copy

Passing the inbound array size so we can use one function for Teuchos and std containers (size vs. length)

References DataTransformModel::expData, and ExperimentData::num_experiments().

Referenced by DataTransformModel::update_expanded_response().

14.56.3.13 void archive_best_config_variables (const **ResultsManager** & *results_db,* const **StrStrSizet** & *iterator_id,* const **Variables** & *vars,* const int & *exp_index,* const int & *num_best,* const int & *best_index*) [protected]

Archive the best configuration variables associated with each model response.

Archive best configuration variables.

References ResultsManager::active(), Variables::inactive_continuous_variable_labels(), Variables::inactive_continuous_variables(), Variables::inactive_discrete_int_variable_labels(), Variables::inactive_discrete_int_variables(), Variables::inactive_discrete_real_variable_labels(), Variables::inactive_discrete_real_variables(), Variables::inactive_discrete_string_variable_labels(), Variables::inactive_discrete_string_variables(), and ResultsManager::insert().

Referenced by DataTransformModel::archive_submodel_responses().

14.56.4 Member Data Documentation

14.56.4.1 **DataTransformModel** ∗ dtModelInstance [static], [protected]

static pointer to this class for use in static callbacks

initialization of static needed by RecastModel

Referenced by DataTransformModel::assign_instance(), DataTransformModel::primary_resp_differencer(), and DataTransformModel::set_mapping().

The documentation for this class was generated from the following files:

- DataTransformModel.hpp
- DataTransformModel.cpp

14.57 DataVariables Class Reference

Handle class for variables specification data.

Public Member Functions

- DataVariables ()

    constructor
- DataVariables (const DataVariables &)

copy constructor
- ∼DataVariables ()
  destructor
- DataVariables operator= (const DataVariables &)
  assignment operator
- bool operator== (const DataVariables &)
  equality operator
- void write (std::ostream &s) const
  write a DataVariables object to an std::ostream
- void read (MPIUnpackBuffer &s)
  read a DataVariables object from a packed MPI buffer
- void write (MPIPackBuffer &s) const
  write a DataVariables object to a packed MPI buffer
- std::shared_ptr< DataVariablesRep > data_rep ()
  return dataVarsRep
- size_t continuous_design ()
  return total number of design variables
- size_t discrete_design ()
  return total number of design variables
- size_t continuous_aleatory_uncertain ()
  return total number of continuous aleatory uncertain variables
- size_t discrete_aleatory_uncertain ()
  return total number of continuous aleatory uncertain variables
- size_t continuous_epistemic_uncertain ()
  return total number of epistemic uncertain variables
- size_t discrete_epistemic_uncertain ()
  return total number of epistemic uncertain variables
- size_t continuous_state ()
  return total number of state variables
- size_t discrete_state ()
  return total number of state variables
- size_t design ()
  return total number of design variables
- size_t aleatory_uncertain ()
  return total number of aleatory uncertain variables
- size_t epistemic_uncertain ()
  return total number of epistemic uncertain variables
- size_t uncertain ()
  return total number of uncertain variables
- size_t state ()
  return total number of state variables
- size_t continuous_variables ()
  return total number of continuous variables
- size_t discrete_variables ()
  return total number of discrete variables
- size_t total_variables ()
  return total number of variables

Static Public Member Functions

- static bool id_compare (const DataVariables &dv, const std::string &id)
  compares the idVariables attribute of DataVariables objects

Private Attributes

- std::shared_ptr< DataVariablesRep > dataVarsRep

    pointer to the body (handle-body idiom)

Friends

- class **ProblemDescDB**
- class **NIDRProblemDescDB**

14.57.1 Detailed Description

Handle class for variables specification data.

The DataVariables class is used to provide a memory management handle for the data in DataVariables-Rep. It is populated by IDRProblemDescDB::variables_kwhandler() and is queried by the ProblemDescDB::get-_<datatype>() functions. A list of DataVariables objects is maintained in ProblemDescDB::dataVariablesList, one for each variables specification in an input file.

The documentation for this class was generated from the following files:

- DataVariables.hpp
- DataVariables.cpp

14.58 DataVariablesRep Class Reference

Body class for variables specification data.

Public Member Functions

- ∼DataVariablesRep ()

    destructor

Public Attributes

- String idVariables

    string identifier for the variables specification data set (from the `id_variables` specification in VarSetId)
- short varsView

    user selection/override of variables view: {DEFAULT,ALL,DESIGN, UNCERTAIN,ALEATORY_UNCERTAIN,EPIST-EMIC_UNCERTAIN,STATE}_VIEW
- short varsDomain

    user selection/override of variables domain: {DEFAULT,MIXED,RELAXED}_DOMAIN
- bool uncertainVarsInitPt

    flag indicating user specification of initial points (for local optimization-based UQ methods) for at least one uncertain variable type
- size_t numContinuousDesVars

    number of continuous design variables (from the `continuous_design` specification in VarDV)
- size_t numDiscreteDesRangeVars

    number of discrete design variables defined by an integer range (from the `discrete_design_range` specification in VarDV)
- size_t numDiscreteDesSetIntVars

number of discrete design variables defined by a set of integers (from the `discrete_design_set` *integer specification in VarDV)*

- size_t numDiscreteDesSetStrVars

  number of discrete design variables defined by a set of strings (from the `discrete_design_set` *string specification in VarDV)*

- size_t numDiscreteDesSetRealVars

  number of discrete design variables defined by a set of reals (from the `discrete_design_set` *real specification in VarDV)*

- size_t numNormalUncVars

  number of normal uncertain variables (from the `normal_uncertain` *specification in VarAUV)*

- size_t numLognormalUncVars

  number of lognormal uncertain variables (from the `lognormal_uncertain` *specification in VarAUV)*

- size_t numUniformUncVars

  number of uniform uncertain variables (from the `uniform_uncertain` *specification in VarAUV)*

- size_t numLoguniformUncVars

  number of loguniform uncertain variables (from the `loguniform_uncertain` *specification in VarAUV)*

- size_t numTriangularUncVars

  number of triangular uncertain variables (from the `triangular_uncertain` *specification in VarAUV)*

- size_t numExponentialUncVars

  number of exponential uncertain variables (from the `exponential_uncertain` *specification in VarAUV)*

- size_t numBetaUncVars

  number of beta uncertain variables (from the `beta_uncertain` *specification in VarAUV)*

- size_t numGammaUncVars

  number of gamma uncertain variables (from the `gamma_uncertain` *specification in VarAUV)*

- size_t numGumbelUncVars

  number of gumbel uncertain variables (from the `gumbel_uncertain` *specification in VarAUV)*

- size_t numFrechetUncVars

  number of frechet uncertain variables (from the `frechet_uncertain` *specification in VarAUV)*

- size_t numWeibullUncVars

  number of weibull uncertain variables (from the `weibull_uncertain` *specification in VarAUV)*

- size_t numHistogramBinUncVars

  number of histogram bin uncertain variables (from the `histogram_bin_uncertain` *specification in VarAUV)*

- size_t numPoissonUncVars

  number of Poisson uncertain variables (from the `poisson_uncertain` *specification in VarAUV)*

- size_t numBinomialUncVars

  number of binomial uncertain variables (from the `binomial_uncertain` *specification in VarAUV)*

- size_t numNegBinomialUncVars

  number of negative binomial uncertain variables (from the `negative_binomial_uncertain` *specification in VarAUV)*

- size_t numGeometricUncVars

  number of geometric uncertain variables (from the `geometric_uncertain` *specification in VarAUV*

- size_t numHyperGeomUncVars

  number of hypergeometric uncertain variables (from the `hypergeometric_uncertain` *specification in VarAUV))*

- size_t numHistogramPtIntUncVars

  number of integer-valued histogram point uncertain variables (from the `histogram_point_uncertain` *specification in VarAUV)*

- size_t numHistogramPtStrUncVars

  number of string-valued histogram point uncertain variables (from the `histogram_point_uncertain` *specification in VarAUV)*

- size_t numHistogramPtRealUncVars

number of real-valued histogram point uncertain variables (from the `histogram_point_uncertain` *specification in VarAUV)*

- size_t numContinuousIntervalUncVars

  number of continuous epistemic interval uncertain variables (from the `continuous_interval_uncertain` *specification in VarEUV)*

- size_t numDiscreteIntervalUncVars

  number of discrete epistemic interval uncertain variables (from the `discrete_interval_uncertain` *specification in VarEUV)*

- size_t numDiscreteUncSetIntVars

  number of discrete epistemic uncertain integer set variables (from the `discrete_uncertain_set` *integer specification in VarEUV)*

- size_t numDiscreteUncSetStrVars

  number of discrete epistemic uncertain string set variables (from the `discrete_uncertain_set` *string specification in VarEUV)*

- size_t numDiscreteUncSetRealVars

  number of discrete epistemic uncertain real set variables (from the `discrete_uncertain_set` *real specification in VarEUV)*

- size_t numContinuousStateVars

  number of continuous state variables (from the `continuous_state` *specification in VarSV)*

- size_t numDiscreteStateRangeVars

  number of discrete state variables defined by an integer range (from the `discrete_state_range` *specification in VarDV)*

- size_t numDiscreteStateSetIntVars

  number of discrete state variables defined by a set of integers (from the `discrete_state_set` *integer specification in VarDV)*

- size_t numDiscreteStateSetStrVars

  number of discrete state variables defined by a set of strings (from the `discrete_state_set` *string specification in VarDV)*

- size_t numDiscreteStateSetRealVars

  number of discrete state variables defined by a set of reals (from the `discrete_state_set` *real specification in VarDV)*

- RealVector continuousDesignVars

  initial values for the continuous design variables array (from the `continuous_design` `initial_point` *specification in VarDV)*

- RealVector continuousDesignLowerBnds

  lower bounds array for the continuous design variables (from the `continuous_design` `lower_bounds` *specification in VarDV)*

- RealVector continuousDesignUpperBnds

  upper bounds array for the continuous design variables (from the `continuous_design` `upper_bounds` *specification in VarDV)*

- StringArray continuousDesignScaleTypes

  scale types array for the continuous design variables (from the `continuous_design` `scale_types` *specification in VarDV)*

- RealVector continuousDesignScales

  scales array for the continuous design variables (from the `continuous_design` `scales` *specification in VarDV)*

- IntVector discreteDesignRangeVars

  initial values for the discrete design variables defined by an integer range (from the `discrete_design_range` `initial_point` *specification in VarDV)*

- IntVector discreteDesignRangeLowerBnds

  lower bounds array for the discrete design variables defined by an integer range (from the `discrete_design_range` `lower_bounds` *specification in VarDV)*

- IntVector discreteDesignRangeUpperBnds

  upper bounds array for the discrete design variables defined by an integer range(from the `discrete_design_range` `upper_bounds` *specification in VarDV)*

- BitArray discreteDesignRangeCat

    is each ddr var strictly categorical (true) or relaxable (false)

- IntVector discreteDesignSetIntVars

    initial values for the discrete design variables defined by an integer set (from the `discrete_design_set` *integer* `initial_point` *specification in VarDV)*

- StringArray discreteDesignSetStrVars

    initial values for the discrete design variables defined by a string set (from the `discrete_design_set` *string* `initial_point` *specification in VarDV)*

- RealVector discreteDesignSetRealVars

    initial values for the discrete design variables defined by a real set (from the `discrete_design_set` *real* `initial_point` *specification in VarDV)*

- IntSetArray discreteDesignSetInt

    complete set of admissible values for each of the discrete design variables defined by an integer set (from the `discrete_design_set` *integer* `set_values` *specification in VarDV)*

- StringSetArray discreteDesignSetStr

    complete set of admissible values for each of the discrete design variables defined by a string set (from the `discrete_design_set` *string* `set_values` *specification in VarDV)*

- RealSetArray discreteDesignSetReal

    complete set of admissible values for each of the discrete design variables defined by a real set (from the `discrete_design_set` *real* `set_values` *specification in VarDV)*

- BitArray discreteDesignSetIntCat

    is each ddsi var strictly categorical (true) or relaxable (false)

- BitArray discreteDesignSetRealCat

    is each ddsr var strictly categorical (true) or relaxable (false)

- RealMatrixArray discreteDesignSetIntAdj

    Adjacency matrices for each of the discrete design variables defined by an integer set (from the `discrete_-design_set` *integer* `categorical adjacency` *specification in VarDV.*

- RealMatrixArray discreteDesignSetStrAdj

    Adjacency matrices for each of the discrete design variables defined by a string set (from the `discrete_design-_set` *string* `adjacency` *specification in VarDV.*

- RealMatrixArray discreteDesignSetRealAdj

    Adjacency matrices for each of the discrete design variables defined by a real set (from the `discrete_design-_set` *real* `categorical adjacency` *specification in VarDV.*

- StringArray continuousDesignLabels

    labels array for the continuous design variables (from the `continuous_design descriptors` *specification in VarDV)*

- StringArray discreteDesignRangeLabels

    labels array for the discrete design variables defined by an integer range (from the `discrete_design_range descriptors` *specification in VarDV)*

- StringArray discreteDesignSetIntLabels

    labels array for the discrete design variables defined by an integer set (from the `discrete_design` *set int* `descriptors` *specification in VarDV)*

- StringArray discreteDesignSetStrLabels

    labels array for the discrete design variables defined by a string set (from the `discrete_design_set` *string* `descriptors` *specification in VarDV)*

- StringArray discreteDesignSetRealLabels

    labels array for the discrete design variables defined by a real set (from the `discrete_design_set` *real;* `descriptors` *specification in VarDV)*

- RealVector normalUncMeans

    means of the normal uncertain variables (from the `means` *specification in VarCAUV_Normal)*

- RealVector normalUncStdDevs

    standard deviations of the normal uncertain variables (from the `std_deviations` *specification in VarCAUV_-Normal)*

- RealVector normalUncLowerBnds

distribution lower bounds for the normal uncertain variables (from the `lower_bounds` *specification in VarCAUV_-Normal)*

- RealVector normalUncUpperBnds

  distribution upper bounds for the normal uncertain variables (from the `upper_bounds` *specification in VarCAUV_-Normal)*

- RealVector normalUncVars

  initial values of the normal uncertain variables (from the `initial_point` *specification in VarCAUV_Normal)*

- RealVector lognormalUncLambdas

  lambdas (means of the corresponding normals) of the lognormal uncertain variables (from the `lambdas` *specification in VarCAUV_Lognormal)*

- RealVector lognormalUncZetas

  zetas (standard deviations of the corresponding normals) of the lognormal uncertain variables (from the `zetas` *specification in VarCAUV_Lognormal)*

- RealVector lognormalUncMeans

  means of the lognormal uncertain variables (from the `means` *specification in VarCAUV_Lognormal)*

- RealVector lognormalUncStdDevs

  standard deviations of the lognormal uncertain variables (from the `std_deviations` *specification in VarCAUV_-Lognormal)*

- RealVector lognormalUncErrFacts

  error factors for the lognormal uncertain variables (from the `error_factors` *specification in VarCAUV_Lognormal)*

- RealVector lognormalUncLowerBnds

  distribution lower bounds for the lognormal uncertain variables (from the `lower_bounds` *specification in VarCAU-V_Lognormal)*

- RealVector lognormalUncUpperBnds

  distribution upper bounds for the lognormal uncertain variables (from the `upper_bounds` *specification in VarCAU-V_Lognormal)*

- RealVector lognormalUncVars

  initial values of the lognormal uncertain variables (from the `initial_point` *specification in VarCAUV_Lognormal)*

- RealVector uniformUncLowerBnds

  distribution lower bounds for the uniform uncertain variables (from the `lower_bounds` *specification in VarCAUV_-Uniform)*

- RealVector uniformUncUpperBnds

  distribution upper bounds for the uniform uncertain variables (from the `upper_bounds` *specification in VarCAUV_-Uniform)*

- RealVector uniformUncVars

  initial values of the uniform uncertain variables (from the `initial_point` *specification in VarCAUV_Uniform)*

- RealVector loguniformUncLowerBnds

  distribution lower bounds for the loguniform uncertain variables (from the `lower_bounds` *specification in VarCAU-V_Loguniform)*

- RealVector loguniformUncUpperBnds

  distribution upper bounds for the loguniform uncertain variables (from the `upper_bounds` *specification in VarCAU-V_Loguniform)*

- RealVector loguniformUncVars

  initial values of the loguniform uncertain variables (from the `initial_point` *specification in VarCAUV_-Loguniform)*

- RealVector triangularUncModes

  modes of the triangular uncertain variables (from the `modes` *specification in VarCAUV_Triangular)*

- RealVector triangularUncLowerBnds

  distribution lower bounds for the triangular uncertain variables (from the `lower_bounds` *specification in VarCAUV-_Triangular)*

- RealVector triangularUncUpperBnds

  distribution upper bounds for the triangular uncertain variables (from the `upper_bounds` *specification in VarCAU-V_Triangular)*

- RealVector triangularUncVars

initial values of the triangular uncertain variables (from the `initial_point` *specification in VarCAUV_Triangular)*

- RealVector exponentialUncBetas

  beta factors for the exponential uncertain variables (from the `betas` *specification in VarCAUV_Exponential)*

- RealVector exponentialUncVars

  initial values of the exponential uncertain variables (from the `initial_point` *specification in VarCAUV_-Exponential)*

- RealVector betaUncAlphas

  alpha factors for the beta uncertain variables (from the `means` *specification in VarCAUV_Beta)*

- RealVector betaUncBetas

  beta factors for the beta uncertain variables (from the `std_deviations` *specification in VarCAUV_Beta)*

- RealVector betaUncLowerBnds

  distribution lower bounds for the beta uncertain variables (from the `lower_bounds` *specification in VarCAUV_Beta)*

- RealVector betaUncUpperBnds

  distribution upper bounds for the beta uncertain variables (from the `upper_bounds` *specification in VarCAUV_Beta)*

- RealVector betaUncVars

  initial values of the beta uncertain variables (from the `initial_point` *specification in VarCAUV_Beta)*

- RealVector gammaUncAlphas

  alpha factors for the gamma uncertain variables (from the `alphas` *specification in VarCAUV_Gamma)*

- RealVector gammaUncBetas

  beta factors for the gamma uncertain variables (from the `betas` *specification in VarCAUV_Gamma)*

- RealVector gammaUncVars

  initial values of the gamma uncertain variables (from the `initial_point` *specification in VarCAUV_Gamma)*

- RealVector gumbelUncAlphas

  alpha factors for the gumbel uncertain variables (from the `alphas` *specification in VarCAUV_Gumbel)*

- RealVector gumbelUncBetas

  beta factors for of the gumbel uncertain variables (from the `betas` *specification in VarCAUV_Gumbel)*

- RealVector gumbelUncVars

  initial values of the gumbel uncertain variables (from the `initial_point` *specification in VarCAUV_Gumbel)*

- RealVector frechetUncAlphas

  alpha factors for the frechet uncertain variables (from the `alphas` *specification in VarCAUV_Frechet)*

- RealVector frechetUncBetas

  beta factors for the frechet uncertain variables (from the `betas` *specification in VarCAUV_Frechet)*

- RealVector frechetUncVars

  initial values of the frechet uncertain variables (from the `initial_point` *specification in VarCAUV_Frechet)*

- RealVector weibullUncAlphas

  alpha factors for the weibull uncertain variables (from the `alphas` *specification in VarCAUV_Weibull)*

- RealVector weibullUncBetas

  beta factors for the weibull uncertain variables (from the `betas` *specification in VarCAUV_Weibull)*

- RealVector weibullUncVars

  initial values of the weibull uncertain variables (from the `initial_point` *specification in VarCAUV_Weibull)*

- RealRealMapArray histogramUncBinPairs

  An array for each real-valued bin-based histogram uncertain variable. Each array entry is a map from a real value to its probability (from the `histogram_bin_uncertain` *specification in VarCAUV_Bin_Histogram; see also continuous_linear variable type in LHS manual). Note: bin widths may be unequal and any (x,c) count specifications are converted to (x,y) ordinates (probability densities) within Vchk_HistogramBinUnc() in the NIDR parser.*

- RealVector histogramBinUncVars

  initial values of the histogram bin uncertain variables (from the `initial_point` *specification in VarCAUV_Bin_-Histogram)*

- RealVector poissonUncLambdas

  lambdas (rate parameter) for the poisson uncertain variables (from the `lambdas` *specification in VarDAUV_Poisson)*

- IntVector poissonUncVars

  initial values of the poisson uncertain variables (from the `initial_point` *specification in VarDAUV_Poisson)*

- BitArray poissonUncCat

  is each poisson var strictly categorical (true) or relaxable (false)
- RealVector binomialUncProbPerTrial

  probabilities per each trial (p) for the binomial uncertain variables from the `prob_per_trial` *specification in VarDAUV_Binomial)*
- IntVector binomialUncNumTrials

  Number of trials (N) for the binomial uncertain variables from the `num_trials` *specification in VarDAUV_Binomial)*
- IntVector binomialUncVars

  initial values of the binomial uncertain variables (from the `initial_point` *specification in VarDAUV_Binomial)*
- BitArray binomialUncCat

  is each binomial var strictly categorical (true) or relaxable (false)
- RealVector negBinomialUncProbPerTrial

  probabilities per each trial (p) for the negative binomial uncertain variables from the `prob_per_trial` *specification in VarDAUV_Negative_Binomial)*
- IntVector negBinomialUncNumTrials

  Number of trials (N) for the negative binomial uncertain variables from the `num_trials` *specification in VarDAUV-_Negative_Binomial)*
- IntVector negBinomialUncVars

  initial values of the negative binomial uncertain variables (from the `initial_point` *specification in VarDAUV_-Negative_Binomial)*
- BitArray negBinomialUncCat

  is each negbinomial var strictly categorical (true) or relaxable (false)
- RealVector geometricUncProbPerTrial

  probabilities per each trial (p) for the geometric uncertain variables from the `prob_per_trial` *specification in VarDAUV_Geometric)*
- IntVector geometricUncVars

  initial values of the geometric uncertain variables (from the `initial_point` *specification in VarDAUV_Geometric)*
- BitArray geometricUncCat

  is each geometric var strictly categorical (true) or relaxable (false)
- IntVector hyperGeomUncTotalPop

  Size of total populations (N) for the hypergeometric uncertain variables from the `total_population` *specification in VarDAUV_Hypergeometric)*
- IntVector hyperGeomUncSelectedPop

  Size of selected populations for the hypergeometric uncertain variables from the `selected_population` *specification in VarDAUV_Hypergeometric)*
- IntVector hyperGeomUncNumDrawn

  Number failed in the selected populations for the hypergeometric variables from the `num_drawn` *specification in VarDAUV_Hypergeometric)*
- IntVector hyperGeomUncVars

  initial values of the hypergeometric uncertain variables (from the `initial_point` *specification in VarDAUV_-Hypergeometric)*
- BitArray hyperGeomUncCat

  is each hypergeom var strictly categorical (true) or relaxable (false)
- IntRealMapArray histogramUncPointIntPairs

  An array for each integer-valued point-based histogram uncertain variable. Each array entry is a map from an integer value to its probability. (See discrete histogram in LHS manual; from the `histogram_point_uncertain` *specification in VarDAUV_Point_Histogram)*
- IntVector histogramPointIntUncVars

  initial values of the real-valued histogram point uncertain variables (from the `initial_point` *specification in VarDAUV_Point_Histogram)*
- BitArray histogramUncPointIntCat

  is each hupi var strictly categorical (true) or relaxable (false)
- StringRealMapArray histogramUncPointStrPairs

An array for each string-valued point-based histogram uncertain variable. Each array entry is a map from a string value to its probability. (See discrete histogram in LHS manual; from the `histogram_point_uncertain` *specification in VarDAUV_Point_Histogram)*

- StringArray histogramPointStrUncVars

  initial values of the real-valued histogram point uncertain variables (from the `initial_point` *specification in VarDAUV_Point_Histogram)*

- RealRealMapArray histogramUncPointRealPairs

  An array for each real-valued point-based histogram uncertain variable. Each array entry is a map from a real value to its probability. (See discrete histogram in LHS manual; from the `histogram_point_uncertain` *specification in VarDAUV_Point_Histogram)*

- RealVector histogramPointRealUncVars

  initial values of the real-valued histogram point uncertain variables (from the `initial_point` *specification in VarDAUV_Point_Histogram)*

- BitArray histogramUncPointRealCat

  is each hupr var strictly categorical (true) or relaxable (false)

- RealSymMatrix uncertainCorrelations

  correlation matrix for all uncertain variables (from the `uncertain_correlation_matrix` *specification in VarAUV_Correlations). This matrix specifies rank correlations for LHS sampling and correlation coefficients (rho_ij = normalized covariance matrix) for other methods.*

- RealRealPairRealMapArray continuousIntervalUncBasicProbs

  Probability values per interval cell per epistemic interval uncertain variable (from the `continuous_interval_uncertain` `interval_probs` *specification in VarCEUV_Interval)*

- RealVector continuousIntervalUncVars

  initial values of the continuous interval uncertain variables (from the `initial_point` *specification in VarCEUV_Interval)*

- IntIntPairRealMapArray discreteIntervalUncBasicProbs

  Probability values per interval cell per epistemic interval uncertain variable (from the `discrete_interval_uncertain` `interval_probs` *specification in VarDIUV)*

- IntVector discreteIntervalUncVars

  initial values of the discrete interval uncertain variables (from the `initial_point` *specification in VarDIUV)*

- BitArray discreteIntervalUncCat

  is each diu var strictly categorical (true) or relaxable (false)

- IntRealMapArray discreteUncSetIntValuesProbs

  complete set of admissible values with associated basic probability assignments for each of the discrete epistemic uncertain variables defined by an integer set (from the `discrete_uncertain_set` *integer* `set_values` *specification in VarDUSIV)*

- IntVector discreteUncSetIntVars

  initial values of the discrete uncertain set integer variables (from the `initial_point` *specification in VarDUSIV)*

- BitArray discreteUncSetIntCat

  is each dusi var strictly categorical (true) or relaxable (false)

- StringRealMapArray discreteUncSetStrValuesProbs

  complete set of admissible values with associated basic probability assignments for each of the discrete epistemic uncertain variables defined by a string set (from the `discrete_uncertain_set` *string* `set_values` *specification in VarDUSIV)*

- StringArray discreteUncSetStrVars

  initial values of the discrete uncertain set integer variables (from the `initial_point` *specification in VarDUSIV)*

- RealRealMapArray discreteUncSetRealValuesProbs

  complete set of admissible values with associated basic probability assignments for each of the discrete epistemic uncertain variables defined by a real set (from the `discrete_uncertain_set_` *eal* `set_values` *specification in VarDUSRV)*

- RealVector discreteUncSetRealVars

  initial values of the discrete uncertain set real variables (from the `initial_point` *specification in VarDUSRV)*

- BitArray discreteUncSetRealCat

  is each dusr var strictly categorical (true) or relaxable (false)

- RealVector continuousStateVars

  initial values for the continuous state variables array (from the `continuous_state` `initial_point` *specification in VarSV)*

- RealVector continuousStateLowerBnds

  lower bounds array for the continuous state variables (from the `continuous_state` `lower_bounds` *specification in VarSV)*

- RealVector continuousStateUpperBnds

  upper bounds array for the continuous state variables (from the `continuous_state` `upper_bounds` *specification in VarSV)*

- IntVector discreteStateRangeVars

  initial values for the discrete state variables defined by an integer range (from the `discrete_state_range` `initial_point` *specification in VarSV)*

- IntVector discreteStateRangeLowerBnds

  lower bounds array for the discrete state variables defined by an integer range (from the `discrete_state_range` `lower_bounds` *specification in VarSV)*

- IntVector discreteStateRangeUpperBnds

  upper bounds array for the discrete state variables defined by an integer range(from the `discrete_state_range` `upper_bounds` *specification in VarSV)*

- BitArray discreteStateRangeCat

  is each dsr var strictly categorical (true) or relaxable (false)

- IntVector discreteStateSetIntVars

  initial values for the discrete state variables defined by an integer set (from the `discrete_state_set` *integer* `initial_point` *specification in VarSV)*

- StringArray discreteStateSetStrVars

  initial values for the discrete state variables defined by a string set (from the `discrete_state_set` *string* `initial_point` *specification in VarSV)*

- RealVector discreteStateSetRealVars

  initial values for the discrete state variables defined by a real set (from the `discrete_state_set` *real* `initial_point` *specification in VarSV)*

- IntSetArray discreteStateSetInt

  complete set of admissible values for each of the discrete state variables defined by an integer set (from the `discrete_state_set` *integer* `set_values` *specification in VarSV)*

- StringSetArray discreteStateSetStr

  complete set of admissible values for each of the discrete state variables defined by a string set (from the `discrete_state_set` *string* `set_values` *specification in VarSV)*

- RealSetArray discreteStateSetReal

  complete set of admissible values for each of the discrete state variables defined by a real set (from the `discrete_state_set` *real* `set_values` *specification in VarSV)*

- BitArray discreteStateSetIntCat

  is each dssi var strictly categorical (true) or relaxable (false)

- BitArray discreteStateSetRealCat

  is each dssr var strictly categorical (true) or relaxable (false)

- StringArray continuousStateLabels

  labels array for the continuous state variables (from the `continuous_state` `descriptors` *specification in VarSV)*

- StringArray discreteStateRangeLabels

  labels array for the discrete state variables defined by an integer range (from the `discrete_state_range` `descriptors` *specification in VarSV)*

- StringArray discreteStateSetIntLabels

  labels array for the discrete state variables defined by an integer set (from the `discrete_state_set` `descriptors` *specification in VarSV)*

- StringArray discreteStateSetStrLabels

  labels array for the discrete state variables defined by a string set (from the `discrete_state_set` `descriptors` *specification in VarSV)*

- StringArray discreteStateSetRealLabels

  labels array for the discrete state variables defined by a real set (from the `discrete_state_set descriptors` *specification in VarSV)*
- IntVector discreteDesignSetIntLowerBnds

  discrete design integer set lower bounds inferred from set values
- IntVector discreteDesignSetIntUpperBnds

  discrete design integer set upper bounds inferred from set values
- StringArray discreteDesignSetStrLowerBnds

  discrete design string set lower bounds inferred from set values
- StringArray discreteDesignSetStrUpperBnds

  discrete design stinr set upper bounds inferred from set values
- RealVector discreteDesignSetRealLowerBnds

  discrete design real set lower bounds inferred from set values
- RealVector discreteDesignSetRealUpperBnds

  discrete design real set upper bounds inferred from set values
- RealVector continuousAleatoryUncVars

  array of values for all continuous aleatory uncertain variables
- RealVector continuousAleatoryUncLowerBnds

  distribution lower bounds for all continuous aleatory uncertain variables (collected from `nuv_lower_bounds`, `lnuv_lower_bounds`, `uuv_lower_bounds`, `luuv_lower_bounds`, `tuv_lower_bounds`, *and* `buv_lower_bounds` *specifications in VarAUV, and derived for gamma, gumbel, frechet, weibull and histogram bin specifications)*
- RealVector continuousAleatoryUncUpperBnds

  distribution upper bounds for all continuous aleatory uncertain variables (collected from `nuv_upper_bounds`, `lnuv_upper_bounds`, `uuv_upper_bounds`, `luuv_upper_bounds`, `tuv_lower_bounds`, *and* `buv_upper_bounds` *specifications in VarAUV, and derived for gamma, gumbel, frechet, weibull and histogram bin specifications)*
- StringArray continuousAleatoryUncLabels

  labels for all continuous aleatory uncertain variables (collected from `nuv_descriptors`, `lnuv_descriptors`, `uuv_descriptors`, `luuv_descriptors`, `tuv_descriptors`, `buv_descriptors`, `gauv_descriptors`, `guuv_descriptors`, `fuv_descriptors`, `wuv_descriptors`, *and* `hbuv_descriptors` *specifications in VarAUV)*
- IntVector discreteIntAleatoryUncVars

  array of values for all discrete integer aleatory uncertain variables
- IntVector discreteIntAleatoryUncLowerBnds

  distribution lower bounds for all discrete integer aleatory uncertain variables
- IntVector discreteIntAleatoryUncUpperBnds

  distribution upper bounds for all discrete integer aleatory uncertain variables
- StringArray discreteIntAleatoryUncLabels

  labels for all discrete integer aleatory uncertain variables
- StringArray discreteStrAleatoryUncVars

  array of values for all discrete string epistemic uncertain variables
- StringArray discreteStrAleatoryUncLowerBnds

  distribution lower bounds for all discrete string epistemic uncertain variables
- StringArray discreteStrAleatoryUncUpperBnds

  distribution upper bounds for all discrete string epistemic uncertain variables
- StringArray discreteStrAleatoryUncLabels

  labels for all discrete string epistemic uncertain variables
- RealVector discreteRealAleatoryUncVars

  array of values for all discrete real aleatory uncertain variables
- RealVector discreteRealAleatoryUncLowerBnds

  distribution lower bounds for all discrete real aleatory uncertain variables
- RealVector discreteRealAleatoryUncUpperBnds

distribution upper bounds for all discrete real aleatory uncertain variables

- StringArray discreteRealAleatoryUncLabels

  labels for all discrete real aleatory uncertain variables
- RealVector continuousEpistemicUncVars

  array of values for all continuous epistemic uncertain variables
- RealVector continuousEpistemicUncLowerBnds

  distribution lower bounds for all continuous epistemic uncertain variables
- RealVector continuousEpistemicUncUpperBnds

  distribution upper bounds for all continuous epistemic uncertain variables
- StringArray continuousEpistemicUncLabels

  labels for all continuous epistemic uncertain variables
- IntVector discreteIntEpistemicUncVars

  array of values for all discrete integer epistemic uncertain variables
- IntVector discreteIntEpistemicUncLowerBnds

  distribution lower bounds for all discrete integer epistemic uncertain variables
- IntVector discreteIntEpistemicUncUpperBnds

  distribution upper bounds for all discrete integer epistemic uncertain variables
- StringArray discreteIntEpistemicUncLabels

  labels for all discrete integer epistemic uncertain variables
- StringArray discreteStrEpistemicUncVars

  array of values for all discrete string epistemic uncertain variables
- StringArray discreteStrEpistemicUncLowerBnds

  distribution lower bounds for all discrete string epistemic uncertain variables
- StringArray discreteStrEpistemicUncUpperBnds

  distribution upper bounds for all discrete string epistemic uncertain variables
- StringArray discreteStrEpistemicUncLabels

  labels for all discrete string epistemic uncertain variables
- RealVector discreteRealEpistemicUncVars

  array of values for all discrete real epistemic uncertain variables
- RealVector discreteRealEpistemicUncLowerBnds

  distribution lower bounds for all discrete real epistemic uncertain variables
- RealVector discreteRealEpistemicUncUpperBnds

  distribution upper bounds for all discrete real epistemic uncertain variables
- StringArray discreteRealEpistemicUncLabels

  labels for all discrete real epistemic uncertain variables
- IntVector discreteStateSetIntLowerBnds

  discrete state integer set lower bounds inferred from set values
- IntVector discreteStateSetIntUpperBnds

  discrete state integer set upper bounds inferred from set values
- StringArray discreteStateSetStrLowerBnds

  discrete state string set lower bounds inferred from set values
- StringArray discreteStateSetStrUpperBnds

  discrete state string set upper bounds inferred from set values
- RealVector discreteStateSetRealLowerBnds

  discrete state real set lower bounds inferred from set values
- RealVector discreteStateSetRealUpperBnds

  discrete state real set upper bounds inferred from set values
- RealVector linearIneqConstraintCoeffs

  coefficient matrix for the linear inequality constraints (from the `linear_inequality_constraint_matrix` *specification in MethodIndControl)*
- RealVector linearIneqLowerBnds

lower bounds for the linear inequality constraints (from the `linear_inequality_lower_bounds` *specification in MethodIndControl)*

- RealVector linearIneqUpperBnds

  upper bounds for the linear inequality constraints (from the `linear_inequality_upper_bounds` *specification in MethodIndControl)*

- StringArray linearIneqScaleTypes

  scaling types for the linear inequality constraints (from the `linear_inequality_scale_types` *specification in MethodIndControl)*

- RealVector linearIneqScales

  scaling factors for the linear inequality constraints (from the `linear_inequality_scales` *specification in MethodIndControl)*

- RealVector linearEqConstraintCoeffs

  coefficient matrix for the linear equality constraints (from the `linear_equality_constraint_matrix` *specification in MethodIndControl)*

- RealVector linearEqTargets

  targets for the linear equality constraints (from the `linear_equality_targets` *specification in MethodIndControl)*

- StringArray linearEqScaleTypes

  scaling types for the linear equality constraints (from the `linear_equality_scale_types` *specification in MethodIndControl)*

- RealVector linearEqScales

  scaling factors for the linear equality constraints (from the `linear_equality_scales` *specification in MethodIndControl)*

Private Member Functions

- DataVariablesRep ()

  default constructor

- void write (std::ostream &s) const

  write a DataVariablesRep object to an std::ostream

- void read (MPIUnpackBuffer &s)

  read a DataVariablesRep object from a packed MPI buffer

- void write (MPIPackBuffer &s) const

  write a DataVariablesRep object to a packed MPI buffer

Friends

- class DataVariables

  the handle class can access attributes of the body class directly

14.58.1 Detailed Description

Body class for variables specification data.

The DataVariablesRep class is used to contain the data from a variables keyword specification. Default values are managed in the DataVariablesRep constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::dataVariablesList is private.

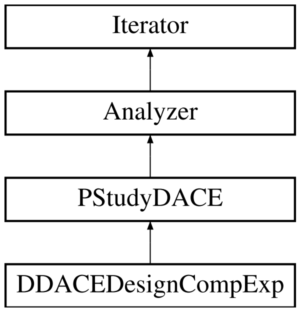
The documentation for this class was generated from the following files:

- DataVariables.hpp
- DataVariables.cpp

14.59 DDACEDesignCompExp Class Reference

Wrapper class for the DDACE design of experiments library.

Inheritance diagram for DDACEDesignCompExp:



Public Member Functions

- DDACEDesignCompExp (ProblemDescDB &problem_db, Model &model)

    primary constructor for building a standard DACE iterator
- DDACEDesignCompExp (Model &model, int samples, int symbols, int seed, unsigned short sampling_-method)

    alternate constructor used for building approximations
- ∼DDACEDesignCompExp ()

    destructor
- bool resize ()

    reinitializes iterator based on new variable size

Protected Member Functions

- void pre_run ()

    pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()

    core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void post_input ()

    read tabular data for post-run mode
- void post_run (std::ostream &s)

    post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- size_t num_samples () const
- void sampling_reset (size_t min_samples, bool all_data_flag, bool stats_flag)

    reset sampling iterator to use at least min_samples
- unsigned short sampling_scheme () const

    return sampling name
- void vary_pattern (bool pattern_flag)

    sets varyPattern in derived classes that support it
- void get_parameter_sets (Model &model)

    Generate one block of numSamples samples (ndim ∗ num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.
- void get_parameter_sets (Model &model, const size_t num_samples, RealMatrix &design_matrix)

    Generate one block of numSamples samples (ndim ∗ num_samples), populating design_matrix.

Private Member Functions

- void compute_main_effects ()

  builds a DDaceMainEffects::OneWayANOVA if mainEffectsFlag is set
- std::shared_ptr< DDaceSamplerBase > create_sampler (Model &model)

  create a DDACE sampler
- void resolve_samples_symbols ()

  convenience function for resolving number of samples and number of symbols from input.

Private Attributes

- unsigned short daceMethod

  oas, lhs, oa_lhs, random, box_behnken, central_composite, or grid
- int samplesSpec

  initial specification of number of samples
- int symbolsSpec

  initial specification of number of symbols
- size_t numSamples

  current number of samples to be evaluated
- size_t numSymbols

  current number of symbols to be used in generating the sample set (inversely related to number of replications)
- const int seedSpec

  the user seed specification for the random number generator (allows repeatable results)
- int randomSeed

  current seed for the random number generator
- bool allDataFlag

  flag which triggers the update of allVars/allResponses for use by Iterator::all_variables() and Iterator::all_responses()
- size_t numDACERuns

  counter for number of executions for this object
- bool varyPattern

  flag for continuing the random number sequence from a previous execution (e.g., for surrogate-based optimization) so that multiple executions are repeatable but not correlated.
- bool mainEffectsFlag

  flag which specifies main effects
- std::vector< std::vector< int > > symbolMapping

  mapping of symbols for main effects calculations

Additional Inherited Members

14.59.1 Detailed Description

Wrapper class for the DDACE design of experiments library.

The DDACEDesignCompExp class provides a wrapper for DDACE, a C++ design of experiments library from the Computational Sciences and Mathematics Research (CSMR) department at Sandia's Livermore CA site. This class uses design and analysis of computer experiments (DACE) methods to sample the design space spanned by the bounds of a Model. It returns all generated samples and their corresponding responses as well as the best sample found.

14.59.2 Constructor & Destructor Documentation

14.59.2.1 DDACEDesignCompExp (ProblemDescDB & *problem_db,* Model & *model*)

primary constructor for building a standard DACE iterator

This constructor is called for a standard iterator built with data from probDescDB.

References Dakota::abort_handler(), DDACEDesignCompExp::daceMethod, DDACEDesignCompExp::mainEffectsFlag, Iterator::maxEvalConcurrency, Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, and DDACEDesignCompExp::numSamples.

14.59.2.2 DDACEDesignCompExp (Model & *model,* int *samples,* int *symbols,* int *seed,* unsigned short *sampling_method*)

alternate constructor used for building approximations

This alternate constructor is used for instantiations on-the-fly, using only the incoming data. No problem description database queries are used.

References Dakota::abort_handler(), Iterator::maxEvalConcurrency, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, DDACEDesignCompExp::numSamples, and DDACEDesignCompExp::resolve_samples_symbols().

14.59.3 Member Function Documentation

14.59.3.1 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

References DDACEDesignCompExp::get_parameter_sets(), Analyzer::get_vbd_parameter_sets(), Iterator::iteratedModel, DDACEDesignCompExp::numSamples, Analyzer::pre_run(), DDACEDesignCompExp::resolve_samples_symbols(), and PStudyDACE::varBasedDecompFlag.

14.59.3.2 void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References DDACEDesignCompExp::allDataFlag, Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, DDACEDesignCompExp::mainEffectsFlag, Analyzer::numLSqTerms, Analyzer::numObjFns, and Iterator::subIteratorFlag.

14.59.3.3 void post_run (std::ostream & *s*) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Analyzer.

References Dakota::abort_handler(), Analyzer::allResponses, Analyzer::allSamples, SensAnalysisGlobal::compute_correlations(), DDACEDesignCompExp::compute_main_effects(), Analyzer::compute_vbd_stats(), DDACEDesignCompExp::create_sampler(), Iterator::iteratedModel, DDACEDesignCompExp::mainEffectsFlag, DDACEDesignCompExp::numSamples, Analyzer::post_run(), PStudyDACE::pStudyDACESensGlobal, DDACEDesignCompExp::seedSpec, Iterator::subIteratorFlag, DDACEDesignCompExp::symbolMapping, and PStudyDACE::varBasedDecompFlag.

14.59.3.4 size_t num_samples ( ) const [inline], [protected], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.

References DDACEDesignCompExp::numSamples.

Referenced by DDACEDesignCompExp::get_parameter_sets().

14.59.3.5 void resolve_samples_symbols ( ) [private]

convenience function for resolving number of samples and number of symbols from input.

This function must define a combination of samples and symbols that is acceptable for a particular sampling algorithm. Users provide requests for these quantities, but this function must enforce any restrictions imposed by the sampling algorithms.

References Dakota::abort_handler(), DDACEDesignCompExp::daceMethod, Analyzer::numContinuousVars, DDACEDesignCompExp::numSamples, DDACEDesignCompExp::numSymbols, and Iterator::submethod_enum_to_string().

Referenced by DDACEDesignCompExp::DDACEDesignCompExp(), DDACEDesignCompExp::post_input(), and DDACEDesignCompExp::pre_run().

The documentation for this class was generated from the following files:

- DDACEDesignCompExp.hpp
- DDACEDesignCompExp.cpp

14.60 DerivInformedPropCovLogitTK< V, M > Class Template Reference

Dakota transition kernel that updates proposal covariance based on derivatives (for logit random walk case)

Inherits TransformedScaledCovMatrixTKGroup< V, M >.

Public Member Functions

- DerivInformedPropCovLogitTK (const char ∗prefix, const QUESO::VectorSet< V, M > &vectorSet, const std::vector< double > &scales, const M &covMatrix, NonDQUESOBayesCalibration ∗queso_instance)

    Constructor for derivative-informed logit proposal covariance.
- virtual ∼DerivInformedPropCovLogitTK ()

    Destructor for derivative-informed logit proposal covariance.
- virtual void **updateTK** () override
- virtual bool covMatrixIsDirty () override

    whether the covariance matrix has been updated
- virtual void cleanCovMatrix () override

    dependent algorithms have taken necessary cleanup actions

Private Attributes

- const QUESO::VectorSet< V, M > & m_vectorSet

  calibration parameter vector set (note: hides base class member)
- bool covIsDirty

  whether we've updated the proposal covariance
- unsigned int chainIndex

  index into current chain position
- NonDQUESOBayesCalibration ∗ nonDQUESOInstance

  Dakota QUESO instance for callbacks.

14.60.1 Detailed Description

template<class V, class M>class Dakota::DerivInformedPropCovLogitTK< V, M >

Dakota transition kernel that updates proposal covariance based on derivatives (for logit random walk case)

The documentation for this class was generated from the following files:

- NonDQUESOBayesCalibration.hpp
- QUESOImpl.hpp
- QUESOImpl.cpp

14.61 DerivInformedPropCovTK< V, M > Class Template Reference

Dakota transition kernel that updates proposal covariance based on derivatives (for random walk case)

Inherits ScaledCovMatrixTKGroup< V, M >.

Public Member Functions

- DerivInformedPropCovTK (const char ∗prefix, const QUESO::VectorSpace< V, M > &vectorSpace, const std::vector< double > &scales, const M &covMatrix, NonDQUESOBayesCalibration ∗queso_instance)

  Constructor for derivative-informed proposal covariance.
- virtual ∼DerivInformedPropCovTK ()

  Destructor for derivative-informed proposal covariance.
- virtual void updateTK () override

  update the transition kernel with new covariance information
- virtual bool covMatrixIsDirty () override

  whether the covariance matrix has been updated
- virtual void cleanCovMatrix () override

  dependent algorithms have taken necessary cleanup actions

Private Attributes

- const QUESO::VectorSpace< V, M > & m_vectorSpace

  calibration parameter vector space (note: hides base class member)
- bool covIsDirty

  whether we've updated the proposal covariance
- unsigned int chainIndex

  index into current chain position
- NonDQUESOBayesCalibration ∗ nonDQUESOInstance

  Dakota QUESO instance for callbacks.

14.61.1 Detailed Description

template< class V, class M >class Dakota::DerivInformedPropCovTK< V, M >

Dakota transition kernel that updates proposal covariance based on derivatives (for random walk case)

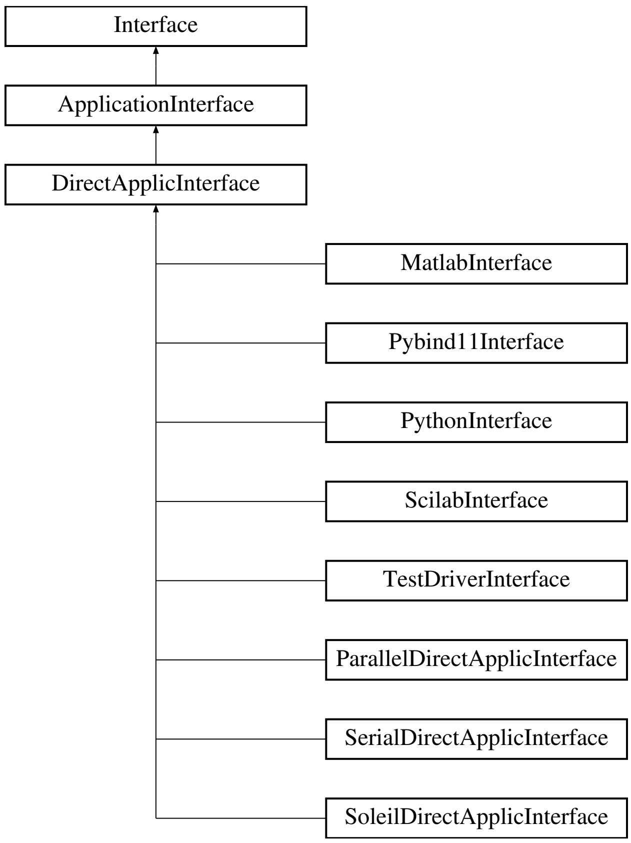
The documentation for this class was generated from the following files:

- NonDQUESOBayesCalibration.hpp
- QUESOImpl.hpp
- QUESOImpl.cpp

14.62 DirectApplicInterface Class Reference

Derived application interface class which spawns simulation codes and testers using direct procedure calls.

Inheritance diagram for DirectApplicInterface:



Public Member Functions

- DirectApplicInterface (const ProblemDescDB &problem_db)

  constructor
- ∼DirectApplicInterface ()

  destructor
- void derived_map (const Variables &vars, const ActiveSet &set, Response &response, int fn_eval_id)

  Called by map() and other functions to execute the simulation in synchronous mode. The portion of performing an evaluation that is specific to a derived class.
- void derived_map_asynch (const ParamResponsePair &pair)

Called by map() and other functions to execute the simulation in asynchronous mode. The portion of performing an asynchronous evaluation that is specific to a derived class.

- void wait_local_evaluations (PRPQueue &prp_queue)

  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version waits for at least one completion.
- void test_local_evaluations (PRPQueue &prp_queue)

  For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version is nonblocking and will return without any completions if none are immediately available.
- int synchronous_local_analysis (int analysis_id)
- const StringArray & analysis_drivers () const

  retrieve the analysis drivers specification for application interfaces
- void init_communicators_checks (int max_eval_concurrency)
- void set_communicators_checks (int max_eval_concurrency)

Protected Member Functions

- virtual int derived_map_if (const Dakota::String &if_name)

  execute the input filter portion of a direct evaluation invocation
- virtual int derived_map_ac (const Dakota::String &ac_name)

  execute an analysis code portion of a direct evaluation invocation
- virtual int derived_map_of (const Dakota::String &of_name)

  execute the output filter portion of a direct evaluation invocation
- virtual void set_local_data (const Variables &vars, const ActiveSet &set)

  convenience function for local test simulators which sets per-evaluation variable and active set attributes; derived classes reimplementing this likely need to invoke the base class API
- virtual void set_local_data (const Response &response)

  convenience function for local test simulators which sets per-evaluation response attributes; derived classes reimplementing this likely need to invoke the base class API
- virtual void set_local_data (const Variables &vars, const ActiveSet &set, const Response &response)

  convenience function for local test simulators which sets per-evaluation variable, active set, and response attributes; derived classes reimplementing this likely need to invoke the base class API
- void overlay_response (Response &response)

  convenience function for local test simulators which overlays response contributions from multiple analyses using MPI_Reduce

Protected Attributes

- String iFilterName

  name of the direct function input filter
- String oFilterName

  name of the direct function output filter
- driver_t iFilterType

  enum type of the direct function input filter
- driver_t oFilterType

  enum type of the direct function output filter
- bool gradFlag

  signals use of fnGrads in direct simulator functions
- bool hessFlag

  signals use of fnHessians in direct simulator functions
- size_t numFns

  number of functions in fnVals

- size_t numVars

    total number of continuous and discrete variables
- size_t numACV

    total number of continuous variables
- size_t numADIV

    total number of discete integer variables
- size_t numADRV

    total number of discete real variables
- size_t numADSV

    total number of discete string variables
- size_t numDerivVars

    number of active derivative variables
- unsigned short localDataView

    bit-wise record of which local data views are active; see enum local_data_t
- RealVector xC

    continuous variables used within direct simulator fns
- IntVector xDI

    discrete int variables used within direct simulator fns
- RealVector xDR

    discrete real variables used within direct simulator fns
- StringMultiArray xDS

    discrete string variables used within direct simulator fns
- StringMultiArray xCLabels

    continuous variable labels
- StringMultiArray xDILabels

    discrete integer variable labels
- StringMultiArray xDRLabels

    discrete real variable labels
- StringMultiArray xDSLabels

    discrete string variable labels
- StringArray xAllLabels

    all variable labels in input spec order
- RealArray metaData

    real-valued metadata
- StringArray metaDataLabels

    labels for optional metadata
- std::map< String, var_t > varTypeMap

    map from variable label to enum
- std::map< String, driver_t > driverTypeMap

    map from driver name to enum
- std::map< var_t, Real > xCM

    map from var_t enum to continuous value
- std::map< var_t, int > xDIM

    map from var_t enum to discrete int value
- std::map< var_t, Real > xDRM

    map from var_t enum to discrete real value
- std::map< var_t, String > xDSM

    map from var_t enum to discrete string val
- std::vector< var_t > varTypeDVV

    var_t enumerations corresponding to DVV components
- std::vector< var_t > xCMLabels

var_t enumerations corresponding to continuous variable labels
- std::vector< var_t > xDIMLabels

    var_t enumerations corresponding to discrete integer variable labels
- std::vector< var_t > xDRMLabels

    var_t enumerations corresponding to discrete real variable labels
- std::vector< var_t > xDSMLabels

    var_t enumerations corresponding to discrete string variable labels
- ShortArray directFnASV

    class scope active set vector
- SizetArray directFnDVV

    class scope derivative variables vector
- RealVector fnVals

    response fn values within direct simulator fns
- RealMatrix fnGrads

    response fn gradients w/i direct simulator fns
- RealSymMatrixArray fnHessians

    response fn Hessians within direct fns
- StringArray analysisDrivers

    the set of analyses within each function evaluation (from the analysis_drivers interface specification)
- std::vector< driver_t > analysisDriverTypes

    conversion of analysisDrivers to driver_t
- size_t analysisDriverIndex

    the index of the active analysis driver within analysisDrivers

Private Member Functions

- void map_labels_to_enum (StringMultiArrayConstView &src, std::vector< var_t > &dest)

    map labels in src to var_t in dest

Private Attributes

- String prevVarsId

    for tracking need to update variables label arrays
- String prevRespId

    for tracking need to update response label arrays

14.62.1 Detailed Description

Derived application interface class which spawns simulation codes and testers using direct procedure calls.

DirectApplicInterface uses a few linkable simulation codes and several internal member functions to perform parameter to response mappings.

14.62.2 Member Function Documentation

14.62.2.1 int synchronous_local_analysis (int *analysis_id*) [inline], [virtual]

This code provides the derived function used by ApplicationInterface::serve_analyses_synch().

Reimplemented from ApplicationInterface.

References DirectApplicInterface::analysisDriverIndex, DirectApplicInterface::analysisDrivers, and DirectApplicInterface::derived_map_ac().

14.62.2.2 void init_communicators_checks (int *max_eval_concurrency*) [inline], [virtual]

Process init issues as warnings since some contexts (e.g., HierarchSurrModel) initialize more configurations than will be used and DirectApplicInterface allows override by derived plug-ins.

Reimplemented from ApplicationInterface.

Reimplemented in Pybind11Interface.

References ApplicationInterface::check_asynchronous(), and ApplicationInterface::check_multiprocessor_-asynchronous().

14.62.2.3 void set_communicators_checks (int *max_eval_concurrency*) [inline], [virtual]

Process run-time issues as hard errors.

Reimplemented from ApplicationInterface.

Reimplemented in SerialDirectApplicInterface, SoleilDirectApplicInterface, ParallelDirectApplicInterface, and Pybind11Interface.

References Dakota::abort_handler(), ApplicationInterface::check_asynchronous(), and ApplicationInterface::check-_multiprocessor_asynchronous().

14.62.2.4 int derived_map_ac (const Dakota::String & *ac_name*) [protected], [virtual]

execute an analysis code portion of a direct evaluation invocation

When a direct analysis/filter is a member function, the (vars,set,response) data does not need to be passed through the API. If, however, non-member analysis/filter functions are added, then pass (vars,set,response) through to the non-member fns:

```
// API declaration
int sim(const Variables& vars, const ActiveSet& set, Response& response);
// use of API within derived_map_ac()
if (ac_name == "sim")
  fail_code = sim(directFnVars, directFnActSet, directFnResponse);
```

Reimplemented in SerialDirectApplicInterface, SoleilDirectApplicInterface, ParallelDirectApplicInterface, and Test-DriverInterface.

References Dakota::abort_handler(), and ApplicationInterface::analysisServerId.

Referenced by DirectApplicInterface::derived_map(), and DirectApplicInterface::synchronous_local_analysis().

The documentation for this class was generated from the following files:

- DirectApplicInterface.hpp
- DirectApplicInterface.cpp

14.63 DiscrepancyCorrection Class Reference

Base class for discrepancy corrections.

Public Member Functions

- DiscrepancyCorrection ()

  default constructor
- DiscrepancyCorrection (Model &surr_model, const SizetSet &surr_fn_indices, short corr_type, short corr_-order, String approx_type="local_taylor", short approx_order=SHRT_MAX)

standard constructor

- DiscrepancyCorrection (const SizetSet &surr_fn_indices, size_t num_fns, size_t num_vars, short corr_type, short corr_order, String approx_type="local_taylor", short approx_order=SHRT_MAX)

  alternate constructor
- ∼DiscrepancyCorrection ()

  destructor
- void initialize (Model &surr_model, const SizetSet &surr_fn_indices, short corr_type, short corr_order, String approx_type="local_taylor", short approx_order=SHRT_MAX)

  initialize the DiscrepancyCorrection data
- void initialize (const SizetSet &surr_fn_indices, size_t num_fns, size_t num_vars, short corr_type, short corr_order, String approx_type="local_taylor", short approx_order=SHRT_MAX)

  initialize the DiscrepancyCorrection data
- void compute (const Variables &vars, const Response &truth_response, const Response &approx_response, bool quiet_flag=false)

  compute the correction required to bring approx_response into agreement with truth_response and store in {add,mult}Corrections
- void compute (const Response &truth_response, const Response &approx_response, Response &discrepancy_response, bool quiet_flag=false)

  compute the correction required to bring approx_response into agreement with truth_response and store in discrepancy_response
- void compute (const VariablesArray &vars_array, const ResponseArray &truth_response_array, const ResponseArray &approx_response, bool quiet_flag=false)

  compute the correction required to bring approx_response into agreement with truth_response as a function of the variables and store in {add,mult}Corrections
- void apply (const Variables &vars, Response &approx_response, bool quiet_flag=false)

  apply the correction computed in compute() to approx_response
- void compute_variance (const VariablesArray &vars_array, RealMatrix &approx_variance, bool quiet_flag=false)

  compute the variance of approx_response
- void correction_type (short corr_type)

  update correctionType
- short correction_type () const

  return correctionType
- void correction_order (short order)

  update correctionOrder
- short correction_order () const

  return correctionOrder
- void data_order (short order)

  update dataOrder
- short data_order () const

  return dataOrder
- bool computed () const

  return correctionComputed
- bool initialized () const

  return initializedFlag

Protected Attributes

- SizetSet surrogateFnIndices

  for mixed response sets, this array specifies the response function subset that is approximated
- bool initializedFlag

  indicates that discrepancy correction instance has been initialized following construction

- short correctionType

  approximation correction approach to be used: NO_CORRECTION, ADDITIVE_CORRECTION, MULTIPLICATIVE-_CORRECTION, or COMBINED_CORRECTION.
- short correctionOrder

  approximation correction order to be used: 0, 1, or 2
- short dataOrder

  order of correction data in 3-bit format: overlay of 1 (value), 2 (gradient), and 4 (Hessian)
- bool correctionComputed

  flag indicating whether or not a correction has been computed and is available for application
- size_t numFns

  total number of response functions (of which surrogateFnIndices may define a subset)
- size_t numVars

  number of continuous variables active in the correction

Private Member Functions

- void initialize (short corr_type, short corr_order, String approx_type, short approx_order)

  initialize types and orders
- void initialize_corrections ()

  internal convenience function shared by overloaded initialize() variants
- bool check_multiplicative (const RealVector &truth_fns, const RealVector &approx_fns)

  define badScalingFlag
- void compute_additive (const Response &truth_response, const Response &approx_response, int index, Real &discrep_fn, RealVector &discrep_grad, RealSymMatrix &discrep_hess)

  internal convenience function for computing additive corrections between truth and approximate responses
- void compute_multiplicative (const Response &truth_response, const Response &approx_response, int index, Real &discrep_fn, RealVector &discrep_grad, RealSymMatrix &discrep_hess)

  internal convenience function for computing multiplicative corrections between truth and approximate responses
- void apply_additive (const Variables &vars, Response &approx_response)

  internal convenience function for applying additive corrections to an approximate response
- void apply_multiplicative (const Variables &vars, Response &approx_response)

  internal convenience function for applying multiplicative corrections to an approximate response
- void apply_additive (const Variables &vars, RealVector &approx_fns)

  internal convenience function for applying additive corrections to a set of response functions
- void apply_multiplicative (const Variables &vars, RealVector &approx_fns)

  internal convenience function for applying multiplicative corrections to a set of response functions
- const Response & search_db (const Variables &search_vars, const ShortArray &search_asv)

  search data_pairs for missing approximation data

Private Attributes

- Pecos::DiscrepancyCalculator discrepCalc

  helper utility for calculating discrepancies
- bool badScalingFlag

  flag used to indicate function values near zero for multiplicative corrections; triggers an automatic switch to additive corrections
- bool computeAdditive

  flag indicating the need for additive correction calculations
- bool computeMultiplicative

  flag indicating the need for multiplicative correction calculations
- String approxType

string indicating the discrepancy approximation type

- short approxOrder

  polynomial order of the discrepancy approximation (basis or trend order)

- bool addAnchor

  flag indicating that data additions are anchor points (for updating local and multipoint approximations)

- SharedApproxData sharedData

  data that is shared among all correction Approximations

- std::vector< Approximation > addCorrections

  array of additive corrections; surrogate models of a model discrepancy function (formed from model differences)

- std::vector< Approximation > multCorrections

  array of multiplicative corrections; surrogate models of a model discrepancy function (formed from model ratios)

- Model surrModel

  shallow copy of the surrogate model instance as returned by Model::surrogate_model() (the DataFitSurrModel or HierarchSurrModel::lowFidelityModel instance)

- RealVector combineFactors

  factors for combining additive and multiplicative corrections. Each factor is the weighting applied to the additive correction and 1.-factor is the weighting applied to the multiplicative correction. The factor value is determined by an additional requirement to match the high fidelity function value at the previous correction point (e.g., previous trust region center). This results in a multipoint correction instead of a strictly local correction.

- Variables correctionPrevCenterPt

  copy of center point from the previous correction cycle

- RealVector truthFnsCenter

  truth function values at the current correction point

- RealVector approxFnsCenter

  Surrogate function values at the current correction point.

- RealMatrix approxGradsCenter

  Surrogate gradient values at the current correction point.

- RealVector truthFnsPrevCenter

  copy of truth function values at center of previous correction cycle

- RealVector approxFnsPrevCenter

  copy of approximate function values at center of previous correction cycle

14.63.1 Detailed Description

Base class for discrepancy corrections.

The DiscrepancyCorrection class provides common functions for computing and applying corrections to approximations.

14.63.2 Member Function Documentation

14.63.2.1 void compute (const **Variables** & *vars,* const **Response** & *truth_response,* const **Response** & *approx_response,* bool *quiet_flag* = `false`)

compute the correction required to bring approx_response into agreement with truth_response and store in {add,mult}Corrections

Compute an additive or multiplicative correction that corrects the approx_response to have 0th-order consistency (matches values), 1st-order consistency (matches values and gradients), or 2nd-order consistency (matches values, gradients, and Hessians) with the truth_response at a single point (e.g., the center of a trust region). The 0th-order, 1st-order, and 2nd-order corrections use scalar values, linear scaling functions, and quadratic scaling functions, respectively, for each response function.

References Response::active_set(), Approximation::add(), DiscrepancyCorrection::addAnchor, DiscrepancyCorrection::addCorrections, DiscrepancyCorrection::apply(), DiscrepancyCorrection::apply_additive(), DiscrepancyCorrection::apply_multiplicative(), DiscrepancyCorrection::approxFnsCenter, DiscrepancyCorrection::approxFnsPrevCenter, DiscrepancyCorrection::approxGradsCenter, DiscrepancyCorrection::badScalingFlag, Approximation::clear_current_active_data(), DiscrepancyCorrection::combineFactors, DiscrepancyCorrection::computeAdditive, DiscrepancyCorrection::computeMultiplicative, Variables::continuous_variables(), Response::copy(), DiscrepancyCorrection::correctionComputed, DiscrepancyCorrection::correctionOrder, DiscrepancyCorrection::correctionPrevCenterPt, DiscrepancyCorrection::correctionType, DiscrepancyCorrection::dataOrder, DiscrepancyCorrection::discrepCalc, Variables::discrete_int_variables(), Variables::discrete_real_variables(), Response::function_-gradient_view(), Response::function_gradients(), Response::function_hessian(), Response::function_value(), Response::function_values(), Model::is_null(), DiscrepancyCorrection::multCorrections, DiscrepancyCorrection::numFns, DiscrepancyCorrection::numVars, ActiveSet::request_values(), DiscrepancyCorrection::sharedData, DiscrepancyCorrection::surrModel, DiscrepancyCorrection::surrogateFnIndices, DiscrepancyCorrection::truthFnsCenter, and DiscrepancyCorrection::truthFnsPrevCenter.

Referenced by DiscrepancyCorrection::compute(), HierarchSurrModel::compute_apply_delta(), DataFitSurrModel::derived_evaluate(), DataFitSurrModel::derived_synchronize(), DataFitSurrModel::derived_synchronize_nowait(), and HierarchSurrModel::single_apply().

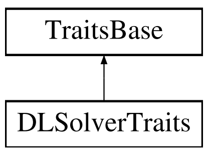
The documentation for this class was generated from the following files:

- DiscrepancyCorrection.hpp
- DiscrepancyCorrection.cpp

14.64 DLSolverTraits Class Reference

A version of TraitsBase specialized for DLSolver.

Inheritance diagram for DLSolverTraits:



Public Member Functions

- DLSolverTraits ()

  default constructor
- virtual ∼DLSolverTraits ()

  destructor
- virtual bool is_derived ()

  A temporary query used in the refactor.
- bool supports_continuous_variables ()

  Return the flag indicating whether method supports continuous variables.
- bool supports_linear_equality ()

  Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()

  Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()

  Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

  Return the flag indicating whether method supports nonlinear inequalities.

- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()

  Return the format used for nonlinear inequality constraints.

14.64.1 Detailed Description

A version of TraitsBase specialized for DLSolver.

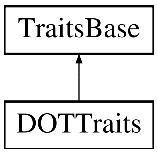
The documentation for this class was generated from the following file:

- DLSolver.hpp

14.65 DOTTraits Class Reference

Wrapper class for the DOT optimization library.

Inheritance diagram for DOTTraits:



Public Member Functions

- DOTTraits ()

  default constructor
- virtual ∼DOTTraits ()

  destructor
- virtual bool is_derived ()

  A temporary query used in the refactor.
- bool supports_continuous_variables ()

  Return the flag indicating whether method supports continuous variables.
- bool supports_linear_equality ()

  Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()

  Return the flag indicating whether method supports linear inequalities.
- LINEAR_INEQUALITY_FORMAT linear_inequality_format ()

  Return the format used for linear inequality constraints.
- bool supports_nonlinear_equality ()

  Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

  Return the flag indicating whether method supports nonlinear inequalities.
- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()

  Return the format used for nonlinear inequality constraints.

14.65.1 Detailed Description

Wrapper class for the DOT optimization library.

The DOTOptimizer class provides a wrapper for DOT, a commercial Fortran 77 optimization library from Vanderplaats Research and Development. It uses a reverse communication mode, which avoids the static member function issues that arise with function pointer designs (see NPSOLOptimizer and SNLLOptimizer).

The user input mappings are as follows: `max_iterations` is mapped into DOT's `ITMAX` parameter within its `IPRM` array, `max_function_evaluations` is implemented directly in the core_run() loop since there is no DOT parameter equivalent, `convergence_tolerance` is mapped into DOT's `DELOBJ` parameter (the relative convergence tolerance) within its `RPRM` array, `output` verbosity is mapped into DOT's `IPRINT` parameter within its function call parameter list (verbose: `IPRINT` = 7; quiet: `IPRINT` = 3), and `optimization_type` is mapped into DOT's `MINMAX` parameter within its function call parameter list. Refer to [Vanderplaats Research and Development, 1995] for information on `IPRM`, `RPRM`, and the DOT function call parameter list. A version of TraitsBase specialized for DOT optimizers

The documentation for this class was generated from the following file:

- DOTOptimizer.hpp

14.66 JEGAOptimizer::Driver Class Reference

A subclass of the JEGA front end driver that exposes the individual protected methods to execute the algorithm.

Inherits Driver.

Public Member Functions

- GeneticAlgorithm ∗ ExtractAllData (const AlgorithmConfig &algConfig)

  Reads all required data from the problem description database stored in the supplied algorithm config.
- DesignOFSortSet PerformIterations (GeneticAlgorithm ∗theGA)

  Performs the required iterations on the supplied GA.
- void DestroyAlgorithm (GeneticAlgorithm ∗theGA)

  Deletes the supplied GA.
- Driver (const ProblemConfig &probConfig)

  Default constructs a Driver.

14.66.1 Detailed Description

A subclass of the JEGA front end driver that exposes the individual protected methods to execute the algorithm.

This is necessary because DAKOTA requires that all problem information be extracted from the problem description DB at the time of Optimizer construction and the front end does it all in the execute algorithm method which must be called in core_run.

14.66.2 Constructor & Destructor Documentation

14.66.2.1 Driver (const ProblemConfig & *probConfig*) [inline]

Default constructs a Driver.

Parameters

probConfig	The definition of the problem to be solved by this Driver whenever ExecuteAlgorithm is called.

The problem can be solved in multiple ways by multiple algorithms even using multiple different evaluators by issuing multiple calls to ExecuteAlgorithm with different AlgorithmConfigs.

14.66.3 Member Function Documentation

14.66.3.1 GeneticAlgorithm* ExtractAllData (const AlgorithmConfig & *algConfig*) [inline]

Reads all required data from the problem description database stored in the supplied algorithm config.

The returned GA is fully configured and ready to be run. It must also be destroyed at some later time. You MUST call DestroyAlgorithm for this purpose. Failure to do so could result in a memory leak and an eventual segmentation fault! Be sure to call DestroyAlgorithm prior to destroying the algorithm config that was used to create it!

This is just here to expose the base class method to users.

Parameters

algConfig	The fully loaded configuration object containing the database of parameters for the algorithm to be run on the known problem.

Returns

The fully configured and loaded GA ready to be run using the PerformIterations method.

Referenced by JEGAOptimizer::core_run().

14.66.3.2 DesignOFSortSet PerformIterations (GeneticAlgorithm * *theGA*) [inline]

Performs the required iterations on the supplied GA.

This includes the calls to AlgorithmInitialize and AlgorithmFinalize and logs some information if appropriate.

This is just here to expose the base class method to users.

Parameters

theGA	The GA on which to perform iterations. This parameter must be non-null.

Returns

The final solutions reported by the supplied GA after all iterations and call to AlgorithmFinalize.

Referenced by JEGAOptimizer::core_run().

14.66.3.3 void DestroyAlgorithm (GeneticAlgorithm * *theGA*) [inline]

Deletes the supplied GA.

Use this method to destroy a GA after all iterations have been run. This method knows if the log associated with the GA was created here and needs to be destroyed as well or not.

This is just here to expose the base class method to users.

Be sure to use this prior to destoying the algorithm config object which contains the target. The GA destructor needs the target to be in tact.

Parameters

theGA	The algorithm that is no longer needed and thus must be destroyed.

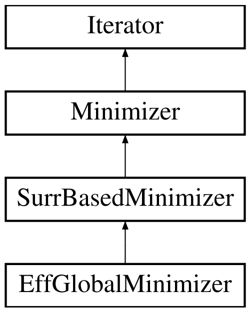
Referenced by JEGAOptimizer::core_run().

The documentation for this class was generated from the following file:

- JEGAOptimizer.cpp

14.67 EffGlobalMinimizer Class Reference

Inheritance diagram for EffGlobalMinimizer:



Public Member Functions

- EffGlobalMinimizer (ProblemDescDB &problem_db, Model &model)

    standard constructor
- EffGlobalMinimizer (Model &model, const String &approx_type, int samples, int seed, bool use_derivs, size_t max_iter, size_t max_eval, Real conv_tol)

    alternate constructor for instantiations "on the fly"
- ∼EffGlobalMinimizer ()

    destructor
- void pre_run ()

    pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()

    core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void post_run (std::ostream &s)

    post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/- Responses and perform final analysis phase in a standalone way
- const Model & algorithm_space_model () const

Private Member Functions

- void initialize_sub_problem (const String &approx_type, int samples, int seed, bool use_derivs, const String &sample_reuse, const String &import_build_points_file=String(), unsigned short import_build_format=TAB-ULAR_ANNOTATED, bool import_build_active_only=false, const String &export_approx_points_file=String(), unsigned short export_approx_format=TABULAR_ANNOTATED)

    shared ctor code for initializing Models and Minimizers for solving an approximate sub-problem
- void initialize_multipliers ()

    initialize Lagrange multipliers in the case of nonlinear constraints

- void check_parallelism ()

  function that checks if model supports asynchronous parallelism
- void build_gp ()

  build initial GP approximations after initial sampling
- void batch_synchronous_ego ()

  synchronous batch-sequential implementation: main function
- void batch_asynchronous_ego ()

  synchronous batch-sequential implementation: main function
- void construct_batch_acquisition (size_t new_acq, size_t new_batch)

  construct a batch of points from performing acquisition cycles
- void construct_batch_exploration (size_t new_expl, size_t new_batch)

  construct a batch of points from performing exploration cycles
- void evaluate_batch (bool rebuild)

  evaluate batch in parallel and replace liar responses
- bool query_batch (bool rebuild)

  perform nonblocking synchronization for parallel evaluation of truth responses and replace liar responses for any completions
- void backfill_batch (size_t new_acq, size_t new_expl)

  backfill any completed truth response evaluations in case of nonblocking synchronization
- void launch_batch ()

  launch all jobs in the variables map queues
- void launch_single (const Variables &vars_star)

  launch a single job
- void process_truth_response_map (const IntResponseMap &truth_resp_map, bool rebuild)

  update approximation data and constraint penalties/multipliers based on new truth data
- void update_variable_maps (const IntResponseMap &truth_resp_map)

  update variable map queues based on completed jobs
- bool converged ()

  check convergence indicators to assess if EGO has converged
- void retrieve_final_results ()

  post-processing: retrieve and export best samples and responses
- void initialize_counters_limits ()

  initialize counters and limits used for assessing convergence
- void update_convergence_counters (const Variables &vars_star, const Response &resp_star)

  update counters used for assessing convergence
- void update_convergence_counters (const Variables &vars_star)

  update counters used for assessing convergence in variables
- void update_convergence_counters (const Response &resp_star)

  update counters used for assessing convergence in response
- void pop_liar_responses ()

  delete all liar responses
- void append_liar (const Variables &vars_star, int liar_id, bool rebuild)

  evaluate and append a liar response
- int extract_id (IntVarsMCIter it, const IntVariablesMap &map)

  manage special value when iterator has advanced to end
- void compute_best_sample ()

  determine meritFnStar from among the GP build data for use in EIF
- void extract_best_sample ()

  extract best solution from among the GP build data for final results
- void extract_qoi_build_data (size_t data_index, RealVector &fn_vals)

  extra response function build data from across the set of QoI

- Real augmented_lagrangian (const RealVector &mean)

  helper for evaluating the value of the augmented Lagrangian merit fn
- void update_constraints (const RealVector &fn_vals)

  update constraint penalties and multipliers for a single response
- void update_constraints (const IntResponseMap &truth_resp_map)

  update constraint penalties and multipliers for a set of responses
- bool empty_queues () const

  helper for checking queued jobs in vars{Acquisition,Exploration}Map
- Real compute_probability_improvement (const RealVector &means, const RealVector &variances)

  probability improvement (PI) function for the EGO PI acquisition function implementation
- Real compute_expected_improvement (const RealVector &means, const RealVector &variances)

  expected improvement (EI) function for the EGO EI acquisition function implementation
- Real compute_lower_confidence_bound (const RealVector &means, const RealVector &variances)

  lower confidence bound (LCB) function for the EGO LCB acquisition function implementation
- Real compute_variances (const RealVector &variances)

  variance function for the EGO MSE acquisition implementation
- RealVector expected_violation (const RealVector &means, const RealVector &variances)

  expected violation function for the constraint functions
- void update_penalty ()

  initialize and update the penaltyParameter
- void debug_print_values (const Variables &vars)

  print mean and variance if debug flag is ON
- void debug_print_dist_counters (Real dist_cv_star)

  print counters if debug flag is ON
- void debug_print_eif_counters (Real eif_star)

  print counters if debug flag is ON
- void debug_plots ()

  DEBUG_PLOTS conditional - output set of samples used to build the GP if problem is 2D.

Static Private Member Functions

- static void PIF_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the objective function in the Expected Improvement (EIF) problem formulation for EGO
- static void EIF_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the objective function in the Expected Improvement (EIF) problem formulation for EGO
- static void LCB_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the objective function in the Lower-Confidence Bound (LCB) problem formulation for EGO
- static void Variances_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  Variance formulation for primary.

Private Attributes

- Model fHatModel

  GP model of response, one approximation per response function.
- Model approxSubProbModel

  recast model which assimilates either (a) mean and variance to solve the max(EIF) sub-problem (used by EIF_objective_eval()) or (b) variance alone for pure exploration (used by Variances_objective_eval())

- Real meritFnStar

  minimum penalized response from among truth build data
- RealVector prevSubProbSoln

  previous solution to EIF approximation sub-problem
- short dataOrder

  order of the data used for surrogate construction, in ActiveSet request vector 3-bit format; user may override responses spec
- int batchSize

  total batch size for parallel EGO
- int batchSizeAcquisition

  number of new sampling points defined from maximizing acquisition function
- int batchSizeExploration

  number of new sampling points defined from maximizing posterior variance
- int batchEvalId

  counter for incrementing evaluation ids to allow synchronization with iteratedModel ids across acquisition and exploration job queues
- IntVariablesMap varsAcquisitionMap

  variable sets for batch evaluation of truth model, accumulated by construct_batch_acquisition()
- IntVariablesMap varsExplorationMap

  variable sets for batch evaluation of truth model, accumulated by construct_batch_exploration()
- bool parallelFlag

  bool flag if model supports asynchronous parallelism
- bool batchAsynch

  algorithm option for fully asynchronous batch updating of the GP
- Real distanceTol

  convergence checkers tolerance convergence on distance between predicted best-so-far samples
- unsigned short eifConvergenceCntr

  counter for convergence in EIF
- unsigned short eifConvergenceLimit

  limit convergence (compared with counter) of EIF
- unsigned short distConvergenceCntr

  counter for distance in input space
- unsigned short distConvergenceLimit

  limit for distance (compared with counter) in input space
- unsigned short globalIterCount

  counter for global iteration

Static Private Attributes

- static EffGlobalMinimizer ∗ effGlobalInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

14.67.1 Detailed Description

The EffGlobalMinimizer class provides an implementation of the Efficient Global Optimization algorithm developed by Jones, Schonlau, & Welch as well as adaptation of the concept to nonlinear least squares.

14.67.2 Member Function Documentation

14.67.2.1 void pre_run ( ) [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Iterator.

References EffGlobalMinimizer::approxSubProbModel, EffGlobalMinimizer::check_parallelism(), EffGlobalMinimizer::initialize_counters_limits(), Model::initialize_mapping(), Iterator::methodPCIter, and SurrBasedMinimizer::miPLIndex.

14.67.2.2 void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References EffGlobalMinimizer::batch_asynchronous_ego(), EffGlobalMinimizer::batch_synchronous_ego(), EffGlobalMinimizer::batchAsynch, EffGlobalMinimizer::build_gp(), and EffGlobalMinimizer::effGlobalInstance.

14.67.2.3 void post_run (std::ostream & *s*) [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Minimizer.

References EffGlobalMinimizer::approxSubProbModel, Model::finalize_mapping(), Minimizer::post_run(), and EffGlobalMinimizer::retrieve_final_results().

14.67.2.4 const Model & algorithm_space_model ( ) const [inline], [virtual]

default definition that gets redefined in selected derived Minimizers

Reimplemented from Minimizer.

References EffGlobalMinimizer::fHatModel.

14.67.2.5 bool query_batch (bool *rebuild*) [private]

perform nonblocking synchronization for parallel evaluation of truth responses and replace liar responses for any completions

query running jobs and process any new completions

References Model::component_parallel_mode(), EffGlobalMinimizer::empty_queues(), EffGlobalMinimizer::fHatModel, Iterator::iteratedModel, EffGlobalMinimizer::process_truth_response_map(), Model::synchronize_nowait(), and EffGlobalMinimizer::update_variable_maps().

Referenced by EffGlobalMinimizer::batch_asynchronous_ego().

14.67.2.6 void compute_best_sample ( ) [private]

determine meritFnStar from among the GP build data for use in EIF

Extract the best merit function from build data through evaluaton of points on fHatModel. This merit fn value is used within the EIF during an approximate sub-problem solve.

References Model::approximation_data(), EffGlobalMinimizer::augmented_lagrangian(), Model::continuous_-variables(), Model::current_response(), Model::evaluate(), EffGlobalMinimizer::fHatModel, Response::function_-values(), EffGlobalMinimizer::meritFnStar, and Minimizer::numFunctions.

Referenced by EffGlobalMinimizer::construct_batch_acquisition().

14.67.2.7 void extract_best_sample ( ) [private]

extract best solution from among the GP build data for final results

Extract the best point from the build data for final results reporting.

References Model::approximation_data(), EffGlobalMinimizer::augmented_lagrangian(), Iterator::bestResponse-Array, Iterator::bestVariablesArray, EffGlobalMinimizer::extract_qoi_build_data(), EffGlobalMinimizer::fHatModel, and Minimizer::numFunctions.

Referenced by EffGlobalMinimizer::retrieve_final_results().

14.67.2.8 Real compute_probability_improvement (const RealVector & *means*, const RealVector & *variances*) [private]

probability improvement (PI) function for the EGO PI acquisition function implementation

Compute the PI acquisition function

References SurrBasedMinimizer::augLagrangeMult, EffGlobalMinimizer::expected_violation(), Iterator::iterated-Model, EffGlobalMinimizer::meritFnStar, Minimizer::numNonlinearConstraints, Minimizer::objective(), SurrBased-Minimizer::penaltyParameter, Model::primary_response_fn_sense(), and Model::primary_response_fn_weights().

Referenced by EffGlobalMinimizer::PIF_objective_eval().

14.67.2.9 Real compute_expected_improvement (const RealVector & *means*, const RealVector & *variances*) [private]

expected improvement (EI) function for the EGO EI acquisition function implementation

Compute the EI acquisition function

References SurrBasedMinimizer::augLagrangeMult, EffGlobalMinimizer::expected_violation(), Iterator::iterated-Model, EffGlobalMinimizer::meritFnStar, Minimizer::numNonlinearConstraints, Minimizer::objective(), SurrBased-Minimizer::penaltyParameter, Model::primary_response_fn_sense(), and Model::primary_response_fn_weights().

Referenced by EffGlobalMinimizer::debug_plots(), and EffGlobalMinimizer::EIF_objective_eval().

14.67.2.10 Real compute_lower_confidence_bound (const RealVector & *means*, const RealVector & *variances*) [private]

lower confidence bound (LCB) function for the EGO LCB acquisition function implementation

Compute the LCB acquisition function

References SurrBasedMinimizer::augLagrangeMult, EffGlobalMinimizer::expected_violation(), Iterator::iterated-Model, Minimizer::numNonlinearConstraints, Minimizer::objective(), SurrBasedMinimizer::penaltyParameter, Model::primary_response_fn_sense(), and Model::primary_response_fn_weights().

Referenced by EffGlobalMinimizer::LCB_objective_eval().

14.67.2.11 Real compute_variances (const RealVector & *variances*) [private]

variance function for the EGO MSE acquisition implementation

Compute the variances

Referenced by EffGlobalMinimizer::Variances_objective_eval().

14.67.2.12 RealVector expected_violation (const RealVector & *means,* const RealVector & *variances*) [private]

expected violation function for the constraint functions

Compute the expected violation for constraints

References Minimizer::bigRealBoundSize, Minimizer::numNonlinearConstraints, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, and SurrBasedMinimizer::origNonlinIneqUpperBnds.

Referenced by EffGlobalMinimizer::compute_expected_improvement(), EffGlobalMinimizer::compute_lower_confidence_bound(), EffGlobalMinimizer::compute_probability_improvement(), and EffGlobalMinimizer::debug_print_values().

14.67.2.13 void PIF_objective_eval (const Variables & *sub_model_vars,* const Variables & *recast_vars,* const Response & *sub_model_response,* Response & *recast_response*) [static], [private]

static function used as the objective function in the Expected Improvement (EIF) problem formulation for EGO

To maximize expected improvement (PI), the approxSubProbMinimizer will minimize -(compute_probability_improvement).

References Response::active_set_request_vector(), Model::approximation_variances(), EffGlobalMinimizer::compute_probability_improvement(), EffGlobalMinimizer::effGlobalInstance, EffGlobalMinimizer::fHatModel, Response::function_value(), and Response::function_values().

14.67.2.14 void EIF_objective_eval (const Variables & *sub_model_vars,* const Variables & *recast_vars,* const Response & *sub_model_response,* Response & *recast_response*) [static], [private]

static function used as the objective function in the Expected Improvement (EIF) problem formulation for EGO

To maximize expected improvement (EI), the approxSubProbMinimizer will minimize -(compute_expected_improvement).

References Response::active_set_request_vector(), Model::approximation_variances(), EffGlobalMinimizer::compute_expected_improvement(), EffGlobalMinimizer::effGlobalInstance, EffGlobalMinimizer::fHatModel, Response::function_value(), and Response::function_values().

Referenced by EffGlobalMinimizer::construct_batch_acquisition().

14.67.2.15 void LCB_objective_eval (const Variables & *sub_model_vars,* const Variables & *recast_vars,* const Response & *sub_model_response,* Response & *recast_response*) [static], [private]

static function used as the objective function in the Lower-Confidence Bound (LCB) problem formulation for EGO

To maximize lower confidence bound (LCB), the approxSubProbMinimizer will minimize -(compute_lower_confidence_bound).

References Response::active_set_request_vector(), Model::approximation_variances(), EffGlobalMinimizer::compute_lower_confidence_bound(), EffGlobalMinimizer::effGlobalInstance, EffGlobalMinimizer::fHatModel, Response::function_value(), and Response::function_values().

14.67.2.16 void Variances_objective_eval (const **Variables** & *sub_model_vars,* const **Variables** & *recast_vars,* const **Response** & *sub_model_response,* **Response** & *recast_response*) [static], [private]

Variance formulation for primary.

To maximize variances, the approxSubProbMinimizer will minimize -(variances).

References Response::active_set_request_vector(), Model::approximation_variances(), EffGlobalMinimizer::compute_variances(), EffGlobalMinimizer::effGlobalInstance, EffGlobalMinimizer::fHatModel, and Response::function_value().

Referenced by EffGlobalMinimizer::construct_batch_exploration().

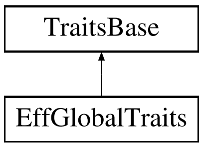
The documentation for this class was generated from the following files:

- EffGlobalMinimizer.hpp
- EffGlobalMinimizer.cpp

14.68 EffGlobalTraits Class Reference

Implementation of Efficient Global Optimization/Least Squares algorithms.

Inheritance diagram for EffGlobalTraits:



Public Member Functions

- EffGlobalTraits ()

  default constructor
- virtual ∼EffGlobalTraits ()

  destructor
- virtual bool is_derived ()

  A temporary query used in the refactor.
- bool supports_continuous_variables ()

  Return the flag indicating whether method supports continuous variables.
- bool supports_nonlinear_equality ()

  Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

  Return the flag indicating whether method supports nonlinear inequalities.

14.68.1 Detailed Description

Implementation of Efficient Global Optimization/Least Squares algorithms.

A version of TraitsBase specialized for efficient global minimizer

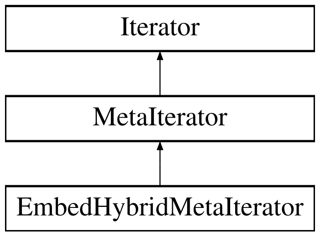
The documentation for this class was generated from the following file:

- EffGlobalMinimizer.hpp

14.69 EmbedHybridMetaIterator Class Reference

Meta-iterator for closely-coupled hybrid iteration, typically involving the embedding of local search methods within global search methods.

Inheritance diagram for EmbedHybridMetaIterator:



Public Member Functions

- EmbedHybridMetaIterator (ProblemDescDB &problem_db)

  standard constructor
- EmbedHybridMetaIterator (ProblemDescDB &problem_db, Model &model)

  alternate constructor
- ∼EmbedHybridMetaIterator ()

  destructor

Protected Member Functions

- void core_run ()

  Performs the hybrid iteration by executing global and local iterators, using a set of models that may vary in fidelity.
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- IntIntPair estimate_partition_bounds ()

  estimate the minimum and maximum partition sizes that can be utilized by this Iterator
- const Variables & variables_results () const

  return the final solution from the embedded hybrid (variables)
- const Response & response_results () const

  return the final solution from the embedded hybrid (response)

Private Attributes

- Iterator globalIterator

  the top-level outer iterator (e.g., global minimizer)
- Model globalModel

  the model employed by the top-level outer iterator
- Iterator localIterator

  the inner iterator (e.g., local minimizer)
- Model localModel

  the model employed by the inner iterator

- bool singlePassedModel

    use of constructor that enforces use of a single passed Model
- Real localSearchProb

    the probability of running a local search refinement within phases of the global minimization for tightly-coupled hybrids

Additional Inherited Members

14.69.1 Detailed Description

Meta-iterator for closely-coupled hybrid iteration, typically involving the embedding of local search methods within global search methods.

This meta-iterator uses multiple methods in close coordination, generally using a local search minimizer repeatedly within a global minimizer (the local search minimizer refines candidate minima which are fed back to the global minimizer).

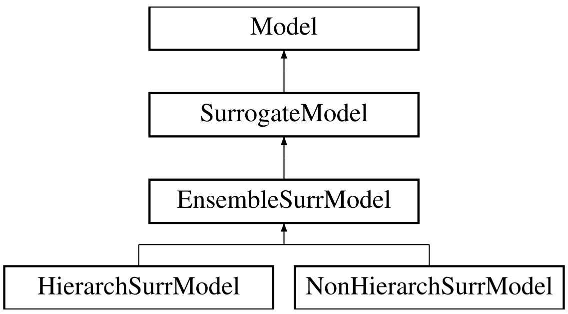
The documentation for this class was generated from the following files:

- EmbedHybridMetaIterator.hpp
- EmbedHybridMetaIterator.cpp

14.70 EnsembleSurrModel Class Reference

Derived model class within the surrogate model branch for managing subordinate models of varying fidelity.

Inheritance diagram for EnsembleSurrModel:



Public Member Functions

- EnsembleSurrModel (ProblemDescDB &problem_db)

    constructor
- ∼EnsembleSurrModel ()

    destructor

Protected Member Functions

- virtual void **derived_synchronize_sequential** (IntResponseMapArray &model_resp_maps_rekey, bool block)=0
- virtual void **derived_synchronize_combine** (IntResponseMapArray &model_resp_maps, IntResponseMap &combined_resp_map)=0
- virtual void **derived_synchronize_combine_nowait** (IntResponseMapArray &model_resp_maps, IntResponseMap &combined_resp_map)=0

- virtual size_t num_approximation_models () const =0

    return the number of models that approximate the truth model
- virtual void assign_default_keys ()=0

    initialize truth and surrogate model keys to default values
- virtual void resize_maps ()=0

    size id_maps and cached_resp_maps arrays according to responseMode
- virtual void resize_response (bool use_virtual_counts=true)=0

    resize currentResponse based on responseMode
- size_t qoi () const

    return number of unique response functions (managing any aggregations)
- void init_model (Model &model)

    initialize model with data that could change once per set of evaluations (e.g., an outer iterator execution), including active variable labels, inactive variable values/bounds/labels, and linear/nonlinear constraint coeffs/bounds
- void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

    set primaryA{C,DI,DS,DR}VarMapIndices, secondaryA{C,DI,DS,DR}VarMapTargets (coming from a higher-level NestedModel context to inform derivative est.)
- const SizetArray & nested_acv1_indices () const

    return primaryACVarMapIndices
- const ShortArray & nested_acv2_targets () const

    return secondaryACVarMapTargets
- short query_distribution_parameter_derivatives () const

    calculate and return derivative composition of final results w.r.t. distribution parameters (none, all, or mixed)
- void check_submodel_compatibility (const Model &sub_model)

    verify compatibility between SurrogateModel attributes and attributes of the submodel (DataFitSurrModel::actualModel or HierarchSurrModel::highFidelityModel)
- const IntResponseMap & derived_synchronize ()
- const IntResponseMap & derived_synchronize_nowait ()
- void stop_servers ()

    Executed by the master to terminate all server operations for a particular model when iteration on the model is complete.
- bool multifidelity () const

    identify if hierarchy is across model forms
- bool multilevel () const

    identify if hierarchy is across resolution levels
- bool multilevel_multifidelity () const

    identify if hierarchy is across both model forms and resolution levels
- bool multifidelity_precedence () const

    return precedence for hierarchy definition, model forms or resolution levels
- void multifidelity_precedence (bool mf_prec, bool update_default=true)

    assign precedence for hierarchy definition (model forms or resolution levels) as determined from algorithm context
- void surrogate_response_mode (short mode)

    set responseMode and pass any bypass request on to the high fidelity model for any lower-level surrogate recursions
- void surrogate_function_indices (const SizetSet &surr_fn_indices)

    (re)set the surrogate index set in SurrogateModel::surrogateFnIndices
- void set_evaluation_reference ()

    set the evaluation counter reference points for the EnsembleSurrModel (request forwarded to truth and surrogate models)
- void init_model_mapped_variables (Model &model)

    initialize model variables that corresponsd to nested mappings that could change once per set of evaluations (e.g., an outer iterator execution)

- void derived_synchronize_competing ()

  called from derived_synchronize() for case of distinct models/interfaces with competing LF/HF job queues
- const String & solution_control_label ()

  helper to select among Variables::all_discrete_{int,string,real}_ variable_labels() for exporting a solution control variable label
- void add_tabular_solution_level_value (Model &model)

  helper to select among Model::solution_level_{int,string,real}_value() for exporting a scalar solution level value

Protected Attributes

- Pecos::ActiveKey truthModelKey

  key defining active model form / resolution level for the truth model
- bool sameModelInstance

  flag indicating that the {low,high}FidelityKey correspond to the same model instance, requiring modifications to updating and evaluation scheduling processes
- bool sameInterfaceInstance

  flag indicating that the models identified by {low,high}FidelityKey employ the same interface instance, requiring modifications to evaluation scheduling processes
- size_t solnCntlAVIndex

  index of solution control variable within all variables
- bool mfPrecedence

  tie breaker for type of model hierarchy when forms and levels are present
- int modeKeyBufferSize

  size of MPI buffer containing responseMode and an aggregated activeKey
- IntIntMapArray modelIdMaps

  map from evaluation ids of truthModel/unorderedModels to EnsembleSurrModel ids
- IntResponseMapArray cachedRespMaps

  maps of responses retrieved in derived_synchronize_nowait() that could not be returned since corresponding response portions were still pending, blocking response aggregation
- SizetArray primaryACVarMapIndices

  "primary" all continuous variable mapping indices flowed down from higher level iteration
- SizetArray primaryADIVarMapIndices

  "primary" all discrete int variable mapping indices flowed down from higher level iteration
- SizetArray primaryADSVarMapIndices

  "primary" all discrete string variable mapping indices flowed down from higher level iteration
- SizetArray primaryADRVarMapIndices

  "primary" all discrete real variable mapping indices flowed down from higher level iteration

Private Member Functions

- bool **test_id_maps** (const IntIntMapArray &id_maps)
- size_t **count_id_maps** (const IntIntMapArray &id_maps)

Additional Inherited Members

14.70.1 Detailed Description

Derived model class within the surrogate model branch for managing subordinate models of varying fidelity.

The EnsembleSurrModel class manages subordinate models of varying fidelity.

14.70.2 Member Function Documentation

14.70.2.1 const IntResponseMap & derived_synchronize ( ) [protected], [virtual]

Blocking retrieval of asynchronous evaluations from LF model, HF model, or both (mixed case). For the LF model portion, apply correction (if active) to each response in the array. derived_synchronize() is designed for the general case where derived_evaluate_nowait() may be inconsistent in its use of low fidelity evaluations, high fidelity evaluations, or both.

Reimplemented from Model.

References EnsembleSurrModel::derived_synchronize_competing(), EnsembleSurrModel::modelIdMaps, EnsembleSurrModel::sameInterfaceInstance, EnsembleSurrModel::sameModelInstance, and SurrogateModel::surrResponseMap.

14.70.2.2 const IntResponseMap & derived_synchronize_nowait ( ) [protected], [virtual]

Nonblocking retrieval of asynchronous evaluations from LF model, HF model, or both (mixed case). For the LF model portion, apply correction (if active) to each response in the map. derived_synchronize_nowait() is designed for the general case where derived_evaluate_nowait() may be inconsistent in its use of actual evals, approx evals, or both.

Reimplemented from Model.

References EnsembleSurrModel::modelIdMaps, and SurrogateModel::surrResponseMap.

Referenced by EnsembleSurrModel::derived_synchronize_competing().

14.70.2.3 void surrogate_response_mode (short *mode*) [inline], [protected], [virtual]

set responseMode and pass any bypass request on to the high fidelity model for any lower-level surrogate recursions

allocate modelIdMaps and cachedRespMaps arrays based on responseMode

Reimplemented from Model.

Reimplemented in HierarchSurrModel.

References EnsembleSurrModel::resize_maps(), EnsembleSurrModel::resize_response(), SurrogateModel::responseMode, Model::surrogate_response_mode(), and Model::truth_model().

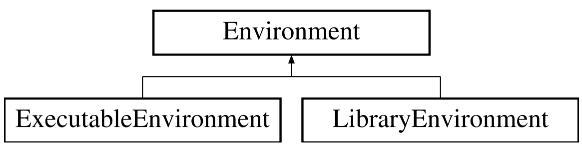
The documentation for this class was generated from the following files:

- EnsembleSurrModel.hpp
- EnsembleSurrModel.cpp

14.71 Environment Class Reference

Base class for the environment class hierarchy.

Inheritance diagram for Environment:



Public Member Functions

- Environment ()

  default constructor: empty envelope
- Environment (int argc, char ∗argv[])

  envelope constructor for ExecutableEnvironment letter
- Environment (ProgramOptions prog_opts)
- Environment (MPI_Comm dakota_mpi_comm, ProgramOptions prog_opts=ProgramOptions())
- Environment (const String &env_type)

  envelope constructor for letter type identifed by String
- Environment (const Environment &env)

  copy constructor
- virtual ∼Environment ()

  destructor
- Environment operator= (const Environment &env)

  assignment operator
- virtual void execute ()

  the run function for the environment: invoke the iterator(s) on the model(s). Called from main.cpp.
- bool check () const

  Print status of check and return true if in a "check" mode, including version and help. Return false if proceeding to a run mode.
- MPIManager & mpi_manager ()

  return mpiManager
- ProgramOptions & program_options ()

  return programOptions
- OutputManager & output_manager ()

  return outputManager
- ParallelLibrary & parallel_library ()

  return parallelLib
- ProblemDescDB & problem_description_db ()

  return probDescDB
- const Variables & variables_results () const

  return the final environment solution (variables)
- const Response & response_results () const

  return the final environment solution (response)
- void exit_mode (const String &mode="exit")

  allow environment clients to set Dakota exit behavior (throw vs. exit)

Protected Member Functions

- Environment (BaseConstructor)

  constructor initializes the base class part of default-constructed letters
- Environment (BaseConstructor, int argc, char ∗argv[])

  constructor initializes the base class part of executable letter classes
- Environment (BaseConstructor, ProgramOptions prog_opts, MPI_Comm dakota_mpi_comm=MPI_COMM_-WORLD)

  constructor initializes the base class part of library letter classes
- void parse (bool check_bcast_database=true, DbCallbackFunctionPtr callback=NULL, void ∗callback_-data=NULL)

  parse inputs, callbacks, and optionally check and broadcast
- void construct ()

Instantiate topLevelIterator.
- void destruct ()

    Deallocate parallel partitioning for topLevelIterator.
- bool **assign_model_pointer** () const

Protected Attributes

- MPIManager mpiManager

    the MPI manager instance
- ProgramOptions programOptions

    the command line options manager
- OutputManager outputManager

    (tagged) output stream manager
- ParallelLibrary parallelLib

    the parallel library instance
- ProblemDescDB probDescDB

    the parser database instance
- Iterator topLevelIterator

    the top level (meta-)iterator
- UsageTracker usageTracker

    tool for Dakota usage tracking (this is a thin wrapper class)

Private Member Functions

- std::shared_ptr< Environment > get_environment (const String &env_type)

    Used by the envelope to instantiate the correct letter class.

Private Attributes

- std::shared_ptr< Environment > environmentRep

    pointer to the letter (initialized only for the envelope)

14.71.1 Detailed Description

Base class for the environment class hierarchy.

The Environment class is the base class for the class hierarchy providing the top level control in DAKOTA. The environment is responsible for creating and managing iterators and models. For memory efficiency and enhanced polymorphism, the environment hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Environment) serves as the envelope and one of the derived classes (selected in Environment::get_environment()) serves as the letter.

14.71.2 Constructor & Destructor Documentation

14.71.2.1 Environment ( )

default constructor: empty envelope

Default envelope constructor. environmentRep is NULL in this case.

14.71.2.2 Environment (int *argc*, char ∗ *argv[]*)

envelope constructor for ExecutableEnvironment letter

Envelope constructor for ExecutableEnvironment. Selection of derived type by get_environment() is not necessary in this case.

References Dakota::abort_handler(), and Environment::environmentRep.

14.71.2.3 Environment (ProgramOptions *prog_opts*)

Envelope constructor for LibraryEnvironment. Selection of derived type by get_environment() is not necessary in this case.

References Dakota::abort_handler(), and Environment::environmentRep.

14.71.2.4 Environment (MPI_Comm *dakota_mpi_comm*, ProgramOptions *prog_opts* = ProgramOptions())

Envelope constructor for LibraryEnvironment. Selection of derived type by get_environment() is not necessary in this case.

References Dakota::abort_handler(), and Environment::environmentRep.

14.71.2.5 Environment (const String & *env_type*)

envelope constructor for letter type identifed by String

Alternate construction by String. Envelope constructor invokes get_environment() which instantiates a derived class letter; the derived constructor selects a BaseConstructor constructor in its initialization list to avoid the recursion of a base class constructor calling get_environment() again.

References Dakota::abort_handler(), and Environment::environmentRep.

14.71.2.6 Environment (const Environment & *env*)

copy constructor

Copy constructor manages sharing of environmentRep.

14.71.2.7 Environment (BaseConstructor) [protected]

constructor initializes the base class part of default-constructed letters

This letter constructor initializes base class data for inherited environments that are default constructed. Since the letter IS the representation, its representation pointer is set to NULL.

Use cases: library with no options, no MPI comm

References ProgramOptions::exit_mode(), Environment::exit_mode(), WorkdirHelper::initialize(), and Environment::programOptions.

14.71.2.8 Environment (BaseConstructor , int *argc*, char ∗ *argv[]*) [protected]

constructor initializes the base class part of executable letter classes

This letter constructor initializes base class data for inherited environments: instantiate/initialize the environment, options, parallel library, and problem description database objects. Since the letter IS the representation, its representation pointer is set to NULL.

Use cases: executable with command-line args

References ProgramOptions::exit_mode(), Environment::exit_mode(), WorkdirHelper::initialize(), and Environment-::programOptions.

14.71.2.9 Environment (BaseConstructor , ProgramOptions *prog_opts*, MPI_Comm *dakota_mpi_comm* = MPI_COMM_WORLD) [protected]

constructor initializes the base class part of library letter classes

This letter constructor initializes base class data for inherited environments. Since the letter IS the representation, its representation pointer is set to NULL.

Use cases: library with program options library with program options and MPI comm

References ProgramOptions::exit_mode(), Environment::exit_mode(), WorkdirHelper::initialize(), and Environment-::programOptions.

14.71.3 Member Function Documentation

14.71.3.1 void exit_mode (const String & *mode* = "exit")

allow environment clients to set Dakota exit behavior (throw vs. exit)

Set the global variable controlling Dakota's exit behavior. Call with no arguments to reset to default behavior.

References Dakota::abort_handler(), and Dakota::abort_mode.

Referenced by Environment::Environment(), and run_dakota_data().

14.71.3.2 void parse (bool *check_bcast_database* = true, DbCallbackFunctionPtr *callback* = NULL, void * *callback_data* = NULL) [protected]

parse inputs, callbacks, and optionally check and broadcast

Parse input file and invoked any callbacks, then optionally check and sync database if check_bcast_database = true

References ProblemDescDB::check_and_broadcast(), ProgramOptions::input_file(), ProgramOptions::input_-string(), ProblemDescDB::parse_inputs(), Environment::probDescDB, and Environment::programOptions.

Referenced by ExecutableEnvironment::ExecutableEnvironment(), and LibraryEnvironment::LibraryEnvironment().

14.71.3.3 std::shared_ptr< Environment > get_environment (const String & *env_type*) [private]

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize environmentRep to the appropriate derived type, as given by the environmentName attribute.

The documentation for this class was generated from the following files:

- DakotaEnvironment.hpp
- DakotaEnvironment.cpp

14.72 NomadOptimizer::Evaluator Class Reference

NOMAD-based Evaluator class.

Inherits Evaluator.

Public Member Functions

- Evaluator (const NOMAD::Parameters &p, Model &model)

    Constructor.
- ∼Evaluator (void)

    Destructor.
- bool eval_x (NOMAD::Eval_Point &x, const NOMAD::Double &h_max, bool &count_eval) const

    Main Evaluation Method.
- bool eval_x (std::list< NOMAD::Eval_Point ∗ > &x, const NOMAD::Double &h_max, std::list< bool > &count-_eval) const

    multi-point variant of evaluator
- void set_constraint_map (int numNomadNonlinearIneqConstraints, int numNomadNonlinearEqConstraints, std::vector< int > constraintMapIndices, std::vector< double > constraintMapMultipliers, std::vector< double > constraintMapOffsets)

    publishes constraint transformation
- void set_surrogate_usage (std::string useSurrogate)

    publishes surrogate usage

Private Member Functions

- void set_variables (const NOMAD::Eval_Point &x) const

    map NOMAD evaluation point to Dakota model
- void eval_model (bool allow_asynch, const NOMAD::Eval_Point &x) const

    evaluate the Dakota model (block or not, but don't collect response)
- void get_responses (const RealVector &ftn_vals, NOMAD::Eval_Point &x) const

    map Dakota model responses to NOMAD evaluation point

Private Attributes

- Model & **_model**
- int **n_cont**
- int **n_disc_int**
- int **n_disc_real**
- int numNomadNonlinearIneqConstr

    Number of nonlinear constraints after put into Nomad format.
- int **numNomadNonlinearEqConstr**
- std::vector< int > constrMapIndices

    map from Dakota constraint number to Nomad constraint number
- std::vector< double > constrMapMultipliers

    multipliers for constraint transformations
- std::vector< double > constrMapOffsets

    offsets for constraint transformations
- std::string useSgte

    defines use of surrogate in NOMAD

14.72.1 Detailed Description

NOMAD-based Evaluator class.

The NOMAD process requires an evaluation step, which calls the Simulation program. In the simplest version of this call, NOMAD executes the black box executable, which proceeds to write a file in a NOMAD-compatible format, which NOMAD reads to continue the process.

Because DAKOTA files are different form NOMAD files, and the simulations processed by DAKOTA already produce DAKOTA-compatible files, we cannot use this method for NOMAD. Instead, we implement the `NomadEvaluator` class, which takes the NOMAD inputs and passes them to DAKOTA's Interface for processing. The evaluator then passes the evaluation Responses into the NOMAD objects for further analysis.

14.72.2 Constructor & Destructor Documentation

14.72.2.1 Evaluator (const NOMAD::Parameters & *p*, Model & *model*)

Constructor.

NOMAD Evaluator Constructor

Parameters

p	NOMAD Parameters object
model	DAKOTA Model object

14.72.3 Member Function Documentation

14.72.3.1 bool eval_x (NOMAD::Eval_Point & *x*, const NOMAD::Double & *h_max*, bool & *count_eval*) const

Main Evaluation Method.

Method that handles the communication between the NOMAD search process and the Black Box Evaluation managed by DAKOTA's Interface.

Parameters

x	Object that contains the points that need to evaluated. Once the evaluation is completed, this object also stores the output back to be read by NOMAD.
h_max	Current value of the barrier parameter. Not used in this implementation.
count_eval	Flag that indicates whether this evaluation counts towards the max number of evaluations, often set to `false` when the evaluation does not meet certain costs during expensive evaluations. Not used in this implementation.

Returns

`true` if the evaluation was successful; `false` otherwise.

References Dakota::get_responses(), and Dakota::set_variables().

The documentation for this class was generated from the following files:

- NomadOptimizer.hpp
- NomadOptimizer.cpp

14.73 JEGAOptimizer::Evaluator Class Reference

An evaluator specialization that knows how to interact with Dakota.

Inherits GeneticAlgorithmEvaluator.

Public Member Functions

- virtual bool Evaluate (DesignGroup &group)

    Does evaluation of each design in group.
- virtual bool Evaluate (Design &des)

    This method cannot be used!!
- virtual std::string GetName () const

    Returns the proper name of this operator.
- virtual std::string GetDescription () const

    Returns a full description of what this operator does and how.
- virtual GeneticAlgorithmOperator ∗ Clone (GeneticAlgorithm &algorithm) const

    Creates and returns a pointer to an exact duplicate of this operator.
- Evaluator (GeneticAlgorithm &algorithm, Model &model)

    Constructs a Evaluator for use by algorithm.
- Evaluator (const Evaluator &copy)

    Copy constructs a Evaluator.
- Evaluator (const Evaluator &copy, GeneticAlgorithm &algorithm, Model &model)

    Copy constructs a Evaluator for use by algorithm.

Static Public Member Functions

- static const std::string & Name ()

    Returns the proper name of this operator.
- static const std::string & Description ()

    Returns a full description of what this operator does and how.

Protected Member Functions

- void SeparateVariables (const Design &from, RealVector &intoCont, IntVector &intoDiscInt, RealVector &intoDiscReal, StringMultiArray &intoDiscString) const

    This method fills intoCont, intoDiscInt and intoDiscReal appropriately using the values of from.
- void RecordResponses (const RealVector &from, Design &into) const

    Records the computed objective and constraint function values into into.
- std::size_t GetNumberNonLinearConstraints () const

    Returns the number of non-linear constraints for the problem.
- std::size_t GetNumberLinearConstraints () const

    Returns the number of linear constraints for the problem.

Private Member Functions

- Evaluator (GeneticAlgorithm &algorithm)

    This constructor has no implementation and cannot be used.

Private Attributes

- Model & _model

    The Model known by this evaluator.

14.73.1 Detailed Description

An evaluator specialization that knows how to interact with Dakota.

This evaluator knows how to use the model to do evaluations both in synchronous and asynchronous modes.

14.73.2 Constructor & Destructor Documentation

14.73.2.1 Evaluator (GeneticAlgorithm & *algorithm*, Model & *model*) [inline]

Constructs a Evaluator for use by *algorithm*.

The optimizer is needed for purposes of variable scaling.

Parameters

algorithm	The GA for which the new evaluator is to be used.
model	The model through which evaluations will be done.

14.73.2.2 Evaluator (const Evaluator & *copy*) [inline]

Copy constructs a Evaluator.

Parameters

copy	The evaluator from which properties are to be duplicated into this.

14.73.2.3 Evaluator (const Evaluator & *copy*, GeneticAlgorithm & *algorithm*, Model & *model*) [inline]

Copy constructs a Evaluator for use by *algorithm*.

The optimizer is needed for purposes of variable scaling.

Parameters

copy	The existing Evaluator from which to retrieve properties.
algorithm	The GA for which the new evaluator is to be used.
model	The model through which evaluations will be done.

14.73.2.4 Evaluator (GeneticAlgorithm & *algorithm*) [private]

This constructor has no implementation and cannot be used.

This constructor can never be used. It is provided so that this operator can still be registered in an operator registry even though it can never be instantiated from there.

Parameters

algorithm	The GA for which the new evaluator is to be used.

14.73.3 Member Function Documentation

14.73.3.1 static const std::string& Name ( ) [inline], [static]

Returns the proper name of this operator.

Returns

The string "DAKOTA JEGA Evaluator".

14.73.3.2 static const std::string& Description ( ) [inline], [static]

Returns a full description of what this operator does and how.

The returned text is:

```
This evaluator uses Sandia's DAKOTA optimization
software to evaluate the passed in Designs.  This
makes it possible to take advantage of the fact that
DAKOTA is designed to run on massively parallel machines.
```

.

Returns

A description of the operation of this operator.

14.73.3.3 void SeparateVariables (const Design & *from,* RealVector & *intoCont,* IntVector & *intoDiscInt,* RealVector & *intoDiscReal,* StringMultiArray & *intoDiscString*) const [protected]

This method fills *intoCont*, *intoDiscInt* and *intoDiscReal* appropriately using the values of *from*.

The discrete integer design variable values are placed in *intoDiscInt*, the discrete real design variable values are placed in *intoDiscReal*, and the continuum are placed into *intoCont*. The values are written into the vectors from the beginning so any previous contents of the vectors will be overwritten.

Parameters

from	The Design class object from which to extract the discrete design variable values.
intoDiscInt	The vector into which to place the extracted discrete integer values.
intoDiscReal	The vector into which to place the extracted discrete real values.
intoCont	The vector into which to place the extracted continuous values.

References JEGAOptimizer::Evaluator::_model, Model::cv(), Model::discrete_int_sets(), Model::discrete_set_-string_values(), Model::div(), Model::drv(), Model::dsv(), and Dakota::set_index_to_value().

14.73.3.4 void RecordResponses (const RealVector & *from,* Design & *into*) const [protected]

Records the computed objective and constraint function values into *into*.

This method takes the response values stored in *from* and properly transfers them into the *into* design.

The response vector *from* is expected to contain values for each objective function followed by values for each non-linear constraint in the order in which the info objects were loaded into the target by the optimizer class.

Parameters

from	The vector of responses to install into *into*.
into	The Design to which the responses belong and into which they must be written.

14.73.3.5 std::size_t GetNumberNonLinearConstraints ( ) const [inline], [protected]

Returns the number of non-linear constraints for the problem.

This is computed by adding the number of non-linear equality constraints to the number of non-linear inequality constraints. These values are obtained from the model.

Returns

The total number of non-linear constraints.

14.73.3.6 std::size_t GetNumberLinearConstraints ( ) const [inline], [protected]

Returns the number of linear constraints for the problem.

This is computed by adding the number of linear equality constraints to the number of linear inequality constraints. These values are obtained from the model.

Returns

The total number of linear constraints.

14.73.3.7 bool Evaluate (DesignGroup & *group*) [virtual]

Does evaluation of each design in *group*.

This method uses the Model known by this class to get Designs evaluated. It properly formats the Design class information in a way that Dakota will understand and then interprets the Dakota results and puts them back into the Design class object. It respects the asynchronous flag in the Model so evaluations may occur synchronously or asynchronously.

Prior to evaluating a Design, this class checks to see if it is marked as already evaluated. If it is, then the evaluation of that Design is not carried out. This is not strictly necessary because Dakota keeps track of evaluated designs and does not re-evaluate. An exception is the case of a population read in from a file complete with responses where Dakota is unaware of the evaluations.

Parameters

group	The group of Design class objects to be evaluated.

Returns

true if all evaluations completed and false otherwise.

14.73.3.8 virtual bool Evaluate (Design & *des*) [inline], [virtual]

This method cannot be used!!

This method does nothing and cannot be called. This is because in the case of asynchronous evaluation, this method would be unable to conform. It would require that each evaluation be done in a synchronous fashion.

Parameters

des	A Design that would be evaluated if this method worked.

Returns

Would return true if the Design were evaluated and false otherwise. Never actually returns here. Issues a fatal error. Otherwise, it would always return false.

14.73.3.9 virtual std::string GetName ( ) const [inline], [virtual]

Returns the proper name of this operator.

Returns

See Name().

14.73.3.10 virtual std::string GetDescription ( ) const [inline], [virtual]

Returns a full description of what this operator does and how.

Returns

See Description().

14.73.3.11 virtual GeneticAlgorithmOperator* Clone (GeneticAlgorithm & *algorithm*) const [inline], [virtual]

Creates and returns a pointer to an exact duplicate of this operator.

Parameters

algorithm	The GA for which the clone is being created.

Returns

A clone of this operator.

14.73.4 Member Data Documentation

14.73.4.1 Model& _model [private]

The Model known by this evaluator.

It is through this model that evaluations will take place.

Referenced by JEGAOptimizer::Evaluator::SeparateVariables().

The documentation for this class was generated from the following file:

- JEGAOptimizer.cpp

14.74 JEGAOptimizer::EvaluatorCreator Class Reference

A specialization of the JEGA::FrontEnd::EvaluatorCreator that creates a new instance of a Evaluator.

Inherits EvaluatorCreator.

Public Member Functions

- virtual GeneticAlgorithmEvaluator * CreateEvaluator (GeneticAlgorithm &alg)

  Overriden to return a newly created Evaluator.
- EvaluatorCreator (Model &theModel)

  Constructs an EvaluatorCreator using the supplied model.

Private Attributes

- Model & _theModel

  The user defined model to be passed to the constructor of the Evaluator.

14.74.1 Detailed Description

A specialization of the JEGA::FrontEnd::EvaluatorCreator that creates a new instance of a Evaluator.

14.74.2 Constructor & Destructor Documentation

14.74.2.1 EvaluatorCreator (Model & *theModel*) [inline]

Constructs an EvaluatorCreator using the supplied model.

Parameters

theModel	The Dakota::Model this creator will pass to the created evaluator.

14.74.3 Member Function Documentation

14.74.3.1 virtual GeneticAlgorithmEvaluator* CreateEvaluator (GeneticAlgorithm & *alg*) [inline], [virtual]

Overriden to return a newly created Evaluator.

The GA will assume ownership of the evaluator so we needn't worry about keeping track of it for destruction. The additional parameters needed by the Evaluator are stored as members of this class at construction time.

Parameters

alg	The GA for which the evaluator is to be created.

Returns

A pointer to a newly created Evaluator.

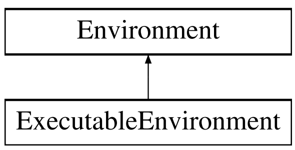
The documentation for this class was generated from the following file:

- JEGAOptimizer.cpp

14.75 ExecutableEnvironment Class Reference

Environment corresponding to execution as a stand-alone application.

Inheritance diagram for ExecutableEnvironment:



Public Member Functions

- ExecutableEnvironment ()

  default constructor
- ExecutableEnvironment (int argc, char *argv[])

  constructor
- ∼ExecutableEnvironment ()

  destructor
- void execute ()

  the run function for the environment: invoke the iterator(s) on the model(s). Called from main.cpp.

Additional Inherited Members

14.75.1 Detailed Description

Environment corresponding to execution as a stand-alone application.

This environment corresponds to a stand-alone executable program, e.g., main.cpp. It sets up the ParallelLibrary, ProgramOptions, and ProblemDescDB objects based on access to command line arguments.

The documentation for this class was generated from the following files:

- ExecutableEnvironment.hpp
- ExecutableEnvironment.cpp

14.76 ExperimentData Class Reference

Interpolation method for interpolating between experimental and model data. I need to work on inputs/outputs to this method. For now, this assumes interpolation of functional data.

Public Member Functions

- ExperimentData ()

    default constructor
- ExperimentData (const ProblemDescDB &prob_desc_db, const SharedResponseData &srd, short output_level)

    typical DB-based constructor
- ExperimentData (size_t num_experiments, size_t num_config_vars, const boost::filesystem::path &data_prefix, const SharedResponseData &srd, const StringArray &variance_types, short output_level, std::string scalarDataFilename="")

    temporary? constructor for testing
- ExperimentData (size_t num_experiments, const SharedVariablesData &svd, const SharedResponseData &srd, const VariablesArray &configVars, const IntResponseMap &all_responses, short output_level)

    Bayesian experimental design constructor. Passed SVD has calibration parameters as active and config vars as inactive variables. Passed configVars have config vars as active.
- void load_data (const std::string &context_message, const Variables &vars_with_state_as_config)

    Load experiments from data files (simple scalar or field)
- void add_data (const SharedVariablesData &svd, const Variables &one_configvars, const Response &one_response)

    Add one data point to the experimental data set. Used for Bayesian experimental design. Passed SVD has calibration parameters as active and config vars as inactive variables. Passed configVars have config vars as active.
- size_t num_experiments () const

    retrieve the number of experiments
- size_t num_total_exppoints () const

    retrieve the total number of experimental data points over all experiments
- size_t num_scalar_primary () const

    retrieve the number of scalars (applies to all experiments)
- size_t num_fields () const

    retrieve the number of fields (applies to all experiments)
- size_t num_config_vars () const

    number of configuration variables
- std::vector< RealVector > config_vars_as_real () const

    values of the configuration variables, 1 RealVector per experiment omits string variables as historically used in NonDBayes

- const std::vector< Variables > & **configuration_variables** () const
- const RealVector & all_data (size_t experiment)

  return contiguous vector of all data (scalar, followed by field) for the specified experiment
- const Response & response (size_t experiment)

  return response for the specified experiment
- void per_exp_length (IntVector &per_length) const

  return the individual sizes of the experimental data lengths (all function values, scalar and field)
- const IntVector & field_lengths (size_t experiment) const

  return the field lengths for specified experiment index
- Real scalar_data (size_t response, size_t experiment)

  retrieve the data value for the given response, for the given experiment
- RealVector field_data_view (size_t response, size_t experiment) const

  retrieve a view of the field data for the given response, for the given experiment
- RealMatrix field_coords_view (size_t response, size_t experiment) const

  retrieve a view of the field data coordinates for the given response, for the given experiment
- void fill_primary_function_labels (StringArray &expanded_labels) const

  populate the passed array with num_total_exppoints labels
- bool variance_type_active (short variance_type) const

  whether the specified variance type (enum value) is present and active
- bool variance_active () const

  whether any variance type is active
- Real apply_covariance (const RealVector &residuals, size_t experiment) const

  apply the covariance responses to compute the triple product v'∗inv(C)∗v for the given experiment
- void apply_covariance_inv_sqrt (const RealVector &residuals, size_t experiment, RealVector &weighted_-residuals) const

  apply inverse sqrt of the covariance to compute weighted residuals
- void apply_covariance_inv_sqrt (const RealMatrix &gradients, size_t experiment, RealMatrix &weighted_-gradients) const

  apply inverse sqrt of the covariance to compute weighted gradients
- void apply_covariance_inv_sqrt (const RealSymMatrixArray &hessians, size_t experiment, RealSymMatrix-Array &weighted_hessians) const

  apply inverse sqrt of the covariance to compute weighted Hessians
- void apply_simulation_error (const RealVector &simulation_error, size_t experiment)

  apply simulation error to experiment data
- void get_main_diagonal (RealVector &diagonal, size_t experiment) const

  return a (copy) vector containing the main diagonal entries of a specified experimental covariance matrix
- void cov_std_deviation (RealVectorArray &std_deviation) const

  get the standard deviation of the observation error process, one vector per experiment
- void cov_as_correlation (RealSymMatrixArray &corr_matrix) const

  get the observation error covariance as a correlation matrix, one vector per experiment
- void covariance (int exp_ind, RealSymMatrix &cov_mat) const

  retrieve an individual covariance entry as a dense matrix
- void form_residuals (const Response &sim_resp, Response &residual_resp) const

  form residuals for all experiments, interpolating if necessary; one simulation response maps to all experiments
- void form_residuals (const Response &sim_resp, const size_t curr_exp, Response &residual_resp) const

  Populate the portion of residual_resp corresponding to experiment curr_exp; the passed simulation response maps only to the specified experiment.
- void form_residuals (const Response &sim_resp, size_t exp_num, const ShortArray &total_asv, size_-t residual_resp_offset, Response &residual_resp) const

  form residuals for an individual experiment, interpolating if necessary
- void recover_model (size_t num_pri_fns, RealVector &model_fns) const

recover original model from the first experiment block in a full set of residuals; works in no interpolation case only (sizes same)

- bool interpolate_flag () const

  flag for interpolation. If 0, no interpolation. If 1, interpolate.

- void interpolate_simulation_data (const Response &sim_resp, size_t exp_num, const ShortArray &total_asv, size_t exp_offset, Response &interp_resp) const

  Interpolate simulation data (values, gradients and hessians) onto the coordinates of the experimental data.

- void scale_residuals (const Response &residual_response, RealVector &scaled_residuals) const

  Apply the experiment data covariance to the residual data (scale functions by Gamma_d^{-1/2}), returning in scaled-_residuals.

- void scale_residuals (Response &residual_response) const

  Apply the experiment data covariance to the residual data in-place (scale functions, gradients, and Hessians by Gamma_d^{-1/2})

- void build_gradient_of_sum_square_residuals (const Response &resp, RealVector &ssr_gradient)

  Build the gradient of the ssr from residuals and function gradients based on the response's active set request vector.

- void build_gradient_of_sum_square_residuals (const Response &resp, const ShortArray &asrv, RealVector &ssr_gradient)

  Build the gradient of the ssr from residuals and function gradients using the passed active set request vector (overrides the response's request vector)

- void build_gradient_of_sum_square_residuals_from_response (const Response &resp, const ShortArray &asrv, int exp_ind, RealVector &ssr_gradient)

  Update the gradient of ssr with the values from the gradient associated with a single experiment.

- void build_gradient_of_sum_square_residuals_from_function_data (const RealMatrix &func_gradients, const RealVector &residuals, RealVector &ssr_gradient, const ShortArray &asrv)

  Construct the gradient of the sum of squares of residuals.

- void build_hessian_of_sum_square_residuals (const Response &resp, RealSymMatrix &ssr_hessian)

  Build the hessian of the ssr from residuals, function gradients and function hessians based on the response's active set request vector.

- void build_hessian_of_sum_square_residuals (const Response &resp, const ShortArray &asrv, RealSymMatrix &ssr_hessian)

  Build the hessian of the ssr from residuals, function gradients and function hessians using the passed active set request vector (overrides the response's request vector)

- void build_hessian_of_sum_square_residuals_from_response (const Response &resp, const ShortArray &asrv, int exp_ind, RealSymMatrix &ssr_hessian)

  Update the hessian of ssr with the values from the hessian associated with a single experiment.

- void build_hessian_of_sum_square_residuals_from_function_data (const RealSymMatrixArray &func_-hessians, const RealMatrix &func_gradients, const RealVector &residuals, RealSymMatrix &ssr_hessian, const ShortArray &asrv)

  Construct the hessian of the sum of squares of residuals.

- void scale_residuals (const RealVector &multipliers, unsigned short multiplier_mode, size_t num_calib_-params, Response &residual_response) const

  in-place scale the residual response (functions, gradients, Hessians) by sqrt(multipliers), according to blocks indicated by multiplier mode

- Real cov_determinant (const RealVector &multipliers, unsigned short multiplier_mode) const

  returns the determinant of (covariance block-scaled by the passed multipliers)

- Real half_log_cov_determinant (const RealVector &multipliers, unsigned short multiplier_mode) const

  returns the log of the determinant of (covariance block-scaled by the passed multipliers)

- void half_log_cov_det_gradient (const RealVector &multipliers, unsigned short multiplier_mode, size_t hyper-_offset, RealVector &gradient) const

  populated the passed gradient with derivatives w.r.t. the hyper-parameter multipliers, starting at hyper_offset (must be sized)

- void half_log_cov_det_hessian (const RealVector &multipliers, unsigned short multiplier_mode, size_t hyper-_offset, RealSymMatrix &hessian) const *populated the passed Hessian with derivatives w.r.t. the hyper-parameter multipliers, starting at hyper_offset (must be sized)*

- StringArray hyperparam_labels (unsigned short multiplier_mode) const

  generate variable labels for the covariance (error) multiplier hyperparams

Protected Member Functions

- ShortArray determine_active_request (const Response &resid_resp) const

  Perform check on the active request vector to make sure it is amenable to interpolation of simulation data and application of apply covariance.
- SizetArray residuals_per_multiplier (unsigned short multiplier_mode) const

  count the number of residuals influenced by each multiplier
- void generate_multipliers (const RealVector &multipliers, unsigned short multiplier_mode, RealVector &expanded_multipliers) const

  Generate a set of multipliers commensurate with the residual size for the total experiment data set. Instead of repeating the loops all over the place, generate an expanded set of multipliers; the conditionals get too complicated otherwise.
- void resid2mult_map (unsigned short multiplier_mode, IntVector &resid2mult_indices) const

  return the index of the multiplier that affects each residual

Private Member Functions

- void initialize (const StringArray &variance_types, const SharedResponseData &srd)

  shared body of constructor initialization
- void parse_sigma_types (const StringArray &sigma_types)

  parse user-provided sigma type strings and populate enums
- void update_data_properties ()

  After constructing or adding data, update properties like experiment lengths, determinant, etc.
- void load_experiment (size_t exp_index, std::ifstream &scalar_data_stream, size_t num_field_sigma_matrices, size_t num_field_sigma_diagonals, size_t num_field_sigma_scalars, size_t num_field_sigma_none, Response &exp_resp)

  Load a single experiment exp_index into exp_resp.
- void read_scalar_sigma (std::ifstream &scalar_data_stream, RealVector &sigma_scalars, IntVector &scalar_map_indices)

  read or default populate the scalar sigma
- RealVector residuals_view (const RealVector &residuals, size_t experiment) const

  Return a view (to allowing updaing in place) of the residuals associated with a given experiment, from a vector contaning residuals from all experiments.
- RealMatrix gradients_view (const RealMatrix &gradients, size_t experiment) const

  Return a view (to allowing updaing in place) of the gradients associated with a given experiment, from a matrix contaning gradients from all experiments.
- RealSymMatrixArray hessians_view (const RealSymMatrixArray &hessians, size_t experiment) const

  Return a view (to allowing updaing in place) of the hessians associated with a given experiment, from an array contaning the hessians from all experiments.

Private Attributes

- bool calibrationDataFlag

  whether the user specified a calibration data block
- size_t numExperiments

  the total number of experiments
- size_t numConfigVars

number of configuration (state) variables to read for each experiment

- UShortArray varianceTypes

  type of variance specified for each variable, one per response group; empty varianceType indicates none specified by user

- Real covarianceDeterminant

  cached product of each experiment covariance's determinant

- Real logCovarianceDeterminant

  cached sum of each experiment covariance's log determinant

- boost::filesystem::path dataPathPrefix

  path to prepend to any data file names

- String scalarDataFilename

  the user-specied scalar data filename

- unsigned short scalarDataFormat

  tabular format of the simple scalar data file; supports TABULAR_NONE, TABULAR_HEADER, TABULAR_EVAL_ID, TABULAR_EXPER_ANNOT

- size_t scalarSigmaPerRow

  number of sigma values to read from each row in simple data file format (calculated from variance types strings

- bool readSimFieldCoords

  whether to read coordinate data files for simulation fields

- SharedResponseData simulationSRD

  archived shared data for use in sizing fields, total functions (historically we read all functions, including constraints, which might not be correct)

- bool interpolateFlag

  flag for interpolation.

- short outputLevel

  output verbosity level

- std::vector< Response > allExperiments

  Vector of numExperiments ExperimentResponses, holding the observed data and error (sigma/covariance) for each experiment.

- std::vector< Variables > allConfigVars

  Vector of numExperiments configurations at which data were gathered; empty if no configurations specified. The inactive state variables are used to store the configuration settings.

- IntVector experimentLengths

  Length of each experiment.

- IntVector expOffsets

  function index offsets for individual experiment data sets

14.76.1 Detailed Description

Interpolation method for interpolating between experimental and model data. I need to work on inputs/outputs to this method. For now, this assumes interpolation of functional data.

As Brian suggested, thsi class has the experimental data (coordinates and RealVectorArray interpolatedResults; The ExperimentData class is used to read and populate data (currently from user-specified files and/or the input spec) relating to experimental (physical observations) data for the purposes of calibration. Such data may include (for example): number of experiments, configuration variables, type of data (scalar vs. functional), treatment of sigma (experimental uncertainties). This class also provides an interpolation capability to interpolate between simulation or experimental data so that the differencing between simulation and experimental data may be performed properly.

14.76.2 Constructor & Destructor Documentation

14.76.2.1 ExperimentData (size_t *num_experiments,* const SharedVariablesData & *svd,* const SharedResponseData & *srd,* const VariablesArray & *config_vars,* const IntResponseMap & *all_responses,* short *output_level*)

Bayesian experimental design constructor. Passed SVD has calibration parameters as active and config vars as inactive variables. Passed configVars have config vars as active.

Used in Hi2Lo Bayesian experimental design; passed config vars are active, but stored here as inactive.

References ExperimentData::allConfigVars, ExperimentData::allExperiments, Response::copy(), SharedResponseData::copy(), SharedVariablesData::copy(), SharedVariablesData::inactive_view(), ExperimentData::numConfigVars, ExperimentData::numExperiments, ExperimentData::outputLevel, SharedResponseData::response_type(), ExperimentData::simulationSRD, Dakota::size_and_fill(), Response::update(), and ExperimentData::update_data_properties().

14.76.3 Member Function Documentation

14.76.3.1 std::vector< RealVector > config_vars_as_real ( ) const

values of the configuration variables, 1 RealVector per experiment omits string variables as historically used in NonDBayes

Skips string vars rather than converting to indices

References ExperimentData::allConfigVars, Dakota::copy_data_partial(), and Dakota::merge_data_partial().

Referenced by NonDGPMSABayesCalibration::fill_experiment_data().

14.76.3.2 void form_residuals (const Response & *sim_resp,* Response & *residual_resp*) const

form residuals for all experiments, interpolating if necessary; one simulation response maps to all experiments

This assumes the souce gradient/Hessian are size less or equal to the destination response, and that the leading part is to be populated.

References ExperimentData::determine_active_request(), ExperimentData::numExperiments, and ExperimentData::per_exp_length().

Referenced by DataTransformModel::archive_submodel_responses(), DataTransformModel::derived_evaluate(), ExperimentData::form_residuals(), DataTransformModel::primary_resp_differencer(), and DataTransformModel::transform_response_map().

14.76.3.3 void form_residuals (const Response & *sim_resp,* size_t *exp_ind,* const ShortArray & *total_asv,* size_t *exp_offset,* Response & *residual_resp*) const

form residuals for an individual experiment, interpolating if necessary

This assumes the souce gradient/Hessian are size less or equal to the destination response, and that the leading part is to be populated.

References ExperimentData::allExperiments, ExperimentData::field_data_view(), Response::field_lengths(), Response::function_gradient_view(), Response::function_gradients(), Response::function_gradients_view(), Response::function_hessian_view(), Response::function_hessians(), Response::function_hessians_view(), Response::function_values(), Response::function_values_view(), ExperimentData::gradients_view(), ExperimentData::hessians_view(), ExperimentData::interpolate_simulation_data(), ExperimentData::interpolateFlag, ExperimentData::num_fields(), ExperimentData::num_scalar_primary(), and ExperimentData::outputLevel.

14.76.3.4 void recover_model (size_t *num_pri_fns,* RealVector & *best_fns*) const

recover original model from the first experiment block in a full set of residuals; works in no interpolation case only (sizes same)

Add the data back to the residual to recover the model, for use in surrogated-based LSQ where DB lookup will fail (need approx eval DB). best_fns contains primary and secondary responses

References Dakota::abort_handler(), ExperimentData::allExperiments, Response::function_value(), ExperimentData::interpolateFlag, SharedResponseData::num_primary_functions(), and Response::shared_data().

14.76.3.5 void build_gradient_of_sum_square_residuals_from_function_data (const RealMatrix & *func_gradients,* const RealVector & *residuals,* RealVector & *ssr_gradient,* const ShortArray & *asrv*)

Construct the gradient of the sum of squares of residuals.

Parameters

func_gradients	A matrix containing the gradients of the residual vector
residuals	A vector of residuals (mismatch between experimental data and the corresponding function values
asrv	The active set request vector

Referenced by ExperimentData::build_gradient_of_sum_square_residuals_from_response().

14.76.3.6 void build_hessian_of_sum_square_residuals_from_function_data (const RealSymMatrixArray & *func_hessians,* const RealMatrix & *func_gradients,* const RealVector & *residuals,* RealSymMatrix & *ssr_hessian,* const ShortArray & *asrv*)

Construct the hessian of the sum of squares of residuals.

Parameters

func_hessians	A list of matrices containing the Hessians of the function elements in the residual vector
func_gradients	A matrix containing the gradients of the residual vector
residuals	A vector of residuals (mismatch between experimental data and the corresponding function values
asrv	The active set request vector

Referenced by ExperimentData::build_hessian_of_sum_square_residuals_from_response().

14.76.3.7 void scale_residuals (const RealVector & *multipliers,* unsigned short *multiplier_mode,* size_t *num_calib_params,* Response & *residual_response*) const

in-place scale the residual response (functions, gradients, Hessians) by sqrt(multipliers), according to blocks indicated by multiplier mode

In-place scaling of residual response by hyper-parameter multipliers

References Dakota::abort_handler(), Response::active_set_request_vector(), Response::function_gradient_view(), Response::function_hessian_view(), Response::function_value(), Response::function_value_view(), ExperimentData::num_total_exppoints(), and ExperimentData::resid2mult_map().

14.76.3.8 Real cov_determinant (const RealVector & *multipliers,* unsigned short *multiplier_mode*) const

returns the determinant of (covariance block-scaled by the passed multipliers)

Determinant of the total covariance used in inference, which has blocks mult_i $*$ I $*$ Cov_i.

References Dakota::abort_handler(), ExperimentData::covarianceDeterminant, ExperimentData::generate_multipliers(), and ExperimentData::num_total_exppoints().

14.76.3.9 Real half_log_cov_determinant (const RealVector & *multipliers,* unsigned short *multiplier_mode*) const

returns the log of the determinant of (covariance block-scaled by the passed multipliers)

Determinant of half the log of total covariance used in inference, which has blocks mult_i ∗ I ∗ Cov_i.

References Dakota::abort_handler(), ExperimentData::generate_multipliers(), ExperimentData::logCovarianceDeterminant, and ExperimentData::num_total_exppoints().

Referenced by NonDBayesCalibration::log_likelihood(), NonDMUQBayesCalibration::print_results(), and NonDQUESOBayesCalibration::print_results().

14.76.3.10 void half_log_cov_det_gradient (const RealVector & *multipliers,* unsigned short *multiplier_mode,* size_t *hyper_offset,* RealVector & *gradient*) const

populated the passed gradient with derivatives w.r.t. the hyper-parameter multipliers, starting at hyper_offset (must be sized)

Compute the gradient of scalar f(m) 0.5∗log(det(mult∗Cov)) w.r.t. mults. Since this is the only use case, we include the 0.5 factor and perform an update in-place.

References ExperimentData::num_total_exppoints(), and ExperimentData::residuals_per_multiplier().

Referenced by NonDBayesCalibration::neg_log_post_resp_mapping().

14.76.3.11 void half_log_cov_det_hessian (const RealVector & *multipliers,* unsigned short *multiplier_mode,* size_t *hyper_offset,* RealSymMatrix & *hessian*) const

populated the passed Hessian with derivatives w.r.t. the hyper-parameter multipliers, starting at hyper_offset (must be sized)

Compute the gradient of scalar f(m) log(det(mult∗Cov)) w.r.t. mults

References ExperimentData::num_total_exppoints(), and ExperimentData::residuals_per_multiplier().

Referenced by NonDBayesCalibration::calculate_evidence(), and NonDBayesCalibration::neg_log_post_resp_mapping().

14.76.3.12 SizetArray residuals_per_multiplier (unsigned short *multiplier_mode*) const [protected]

count the number of residuals influenced by each multiplier

Calculate how many residuals each multiplier affects

References ExperimentData::allExperiments, SharedResponseData::num_field_response_groups(), ExperimentData::num_fields(), SharedResponseData::num_response_groups(), SharedResponseData::num_scalar_primary(), ExperimentData::numExperiments, and ExperimentData::simulationSRD.

Referenced by ExperimentData::half_log_cov_det_gradient(), and ExperimentData::half_log_cov_det_hessian().

14.76.3.13 void parse_sigma_types (const StringArray & *sigma_types*) [private]

parse user-provided sigma type strings and populate enums

Validate user-provided sigma specifcation. User can specify 0, 1, or num_response_groups sigmas. If specified, sigma types must be the same for all scalar responses.

References Dakota::abort_handler(), SharedResponseData::num_field_response_groups(), SharedResponseData::num_scalar_primary(), ExperimentData::scalarDataFilename, ExperimentData::scalarSigmaPerRow, ExperimentData::simulationSRD, and ExperimentData::varianceTypes.

Referenced by ExperimentData::initialize().

14.76.3.14 void load_experiment (size_t *exp_index,* std::ifstream & *scalar_data_stream,* size_t *num_field_sigma_matrices,* size_t *num_field_sigma_diagonals,* size_t *num_field_sigma_scalars,* size_t *num_field_sigma_none,* Response & *exp_resp*) [private]

Load a single experiment exp_index into exp_resp.

Load an experiment from a mixture of legacy format data and field data format files

References Dakota::abort_handler(), ExperimentData::dataPathPrefix, Response::field_coords(), Response::field_group_labels(), ExperimentData::field_lengths(), Response::field_lengths(), Response::field_values(), Response::function_labels(), Response::function_value(), Dakota::is_matrix_symmetric(), SharedResponseData::num_field_response_groups(), ExperimentData::num_fields(), SharedResponseData::num_scalar_primary(), ExperimentData::numExperiments, Dakota::read_coord_values(), Dakota::read_covariance(), Dakota::read_field_values(), ExperimentData::read_scalar_sigma(), ExperimentData::scalarDataFilename, ExperimentData::scalarSigmaPerRow, Response::set_full_covariance(), ExperimentData::simulationSRD, and ExperimentData::varianceTypes.

Referenced by ExperimentData::load_data().

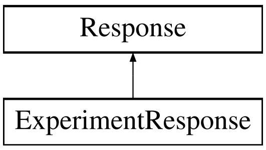
The documentation for this class was generated from the following files:

- ExperimentData.hpp
- ExperimentData.cpp

14.77 ExperimentResponse Class Reference

Container class for response functions and their derivatives. ExperimentResponse provides the body class.

Inheritance diagram for ExperimentResponse:



Public Member Functions

- ExperimentResponse ()
  default constructor
- ExperimentResponse (const Variables &vars, const ProblemDescDB &problem_db)
  standard constructor built from problem description database
- ExperimentResponse (const SharedResponseData &srd, const ActiveSet &set)
  alternate constructor that shares a SharedResponseData instance
- ExperimentResponse (const SharedResponseData &srd)
  alternate constructor that shares a SharedResponseData instance
- ExperimentResponse (const ActiveSet &set)
  alternate constructor using limited data
- ∼ExperimentResponse ()
  destructor
- void set_scalar_covariance (RealVector &scalars) override
  method to set the covariance matrix defined for ExperimentResponse
- const ExperimentCovariance & experiment_covariance () const override
  retrieve the ExperimentCovariance structure
- void set_full_covariance (std::vector< RealMatrix > &matrices, std::vector< RealVector > &diagonals, RealVector &scalars, IntVector matrix_map_indices, IntVector diagonal_map_indices, IntVector scalar_map_indices) override

method to set the full covariance matrices for ExperimentResponse

- Real apply_covariance (const RealVector &residual) const override

  method to compute the triple product v'∗inv(C)∗v.

- void apply_covariance_inv_sqrt (const RealVector &residuals, RealVector &weighted_residuals) const override

  method to compute (v'∗inv(C)^1/2), to compute weighted residual

- void **apply_covariance_inv_sqrt** (const RealMatrix &gradients, RealMatrix &weighted_gradients) const override
- void **apply_covariance_inv_sqrt** (const RealSymMatrixArray &hessians, RealSymMatrixArray &weighted_hessians) const override
- void **get_covariance_diagonal** (RealVector &diagonal) const override
- Real covariance_determinant () const override

  covariance determinant for this experiment (default 1.0)

- Real log_covariance_determinant () const override

  log covariance determinant for this experiment (default 0.0)

Protected Member Functions

- void copy_rep (std::shared_ptr< Response > source_resp_rep) override

  Specialization of copy_rep; pulls base class data as well as derived specific data from the source rep into the this object.

Private Attributes

- ExperimentCovariance expDataCovariance

  sigma terms...

Additional Inherited Members

14.77.1 Detailed Description

Container class for response functions and their derivatives. ExperimentResponse provides the body class.

The ExperimentResponse class is the "representation" of the response container class. It is the "body" portion of the "handle-body idiom" (see Coplien "Advanced C++", p. 58). The handle class (Response) provides for memory efficiency in management of multiple response objects through reference counting and representation sharing. The body class (ExperimentResponse) actually contains the response data (functionValues, functionGradients, functionHessians, etc.). The representation is hidden in that an instance of ExperimentResponse may only be created by Response. Therefore, programmers create instances of the Response handle class, and only need to be aware of the handle/body mechanisms when it comes to managing shallow copies (shared representation) versus deep copies (separate representation used for history mechanisms).

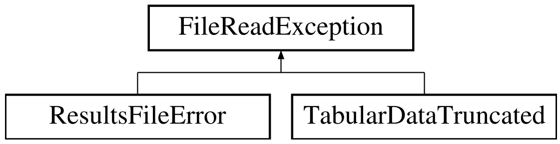
The documentation for this class was generated from the following files:

- ExperimentResponse.hpp
- ExperimentResponse.cpp

14.78 FileReadException Class Reference

base class for Dakota file read exceptions (to allow catching both tabular and general file truncation issues)

Inheritance diagram for FileReadException:



Public Member Functions

- **FileReadException** (const std::string &msg)

14.78.1 Detailed Description

base class for Dakota file read exceptions (to allow catching both tabular and general file truncation issues)

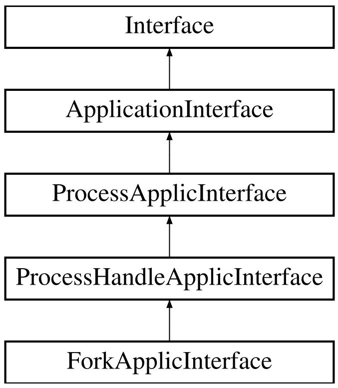
The documentation for this class was generated from the following file:

- dakota_global_defs.hpp

14.79 ForkApplicInterface Class Reference

Derived application interface class which spawns simulation codes using fork/execvp/waitpid.

Inheritance diagram for ForkApplicInterface:



Public Member Functions

- ForkApplicInterface (const ProblemDescDB &problem_db)

    constructor
- ∼ForkApplicInterface ()

    destructor

Protected Member Functions

- void wait_local_evaluation_sequence (PRPQueue &prp_queue)

    version of wait_local_evaluations() managing of set of individual asynchronous evaluations
- void test_local_evaluation_sequence (PRPQueue &prp_queue)

    version of test_local_evaluations() managing of set of individual asynchronous evaluations
- pid_t create_analysis_process (bool block_flag, bool new_group)

spawn a child process for an analysis component within an evaluation using fork()/execvp() and wait for completion using waitpid() if block_flag is true

- size_t wait_local_analyses ()

  wait for asynchronous analyses on the local processor, completing at least one job
- size_t test_local_analyses_send (int analysis_id)

  test for asynchronous analysis completions on the local processor and return results for any completions by sending messages
- void join_evaluation_process_group (bool new_group)

  create (if new_group) and join the process group for asynch evaluations
- void join_analysis_process_group (bool new_group)

  create (if new_group) and join the process group for asynch analyses
- void evaluation_process_group_id (pid_t pgid)

  set evalProcGroupId
- pid_t evaluation_process_group_id () const

  return evalProcGroupId
- void analysis_process_group_id (pid_t pgid)

  set analysisProcGroupId
- pid_t analysis_process_group_id () const

  return analysisProcGroupId
- pid_t wait_evaluation (bool block_flag)

  process all available completions within the evaluation process group; if block_flag = true, wait for at least one completion
- pid_t wait_analysis (bool block_flag)

  process all available completions within the analysis process group; if block_flag = true, wait for at least one completion
- void check_group (int err, pid_t proc_group_id)

  check the exit status of setpgid and abort if an error code was returned

Private Member Functions

- pid_t wait (pid_t proc_group_id, std::map$<$ pid_t, int $>$ &process_id_map, bool block_flag)

  core code used by wait_{evaluation,analysis}()
- void join_process_group (pid_t &process_group_id, bool new_group)

  core code used by join_{evaluation,analysis}_process_group()

Private Attributes

- pid_t evalProcGroupId

  the process group id used to identify a set of child evaluation processes used by this interface instance (to distinguish from other interface instances that could be running at the same time)
- pid_t analysisProcGroupId

  the process group id used to identify a set of child analysis processes used by this interface instance (to distinguish from other interface instances that could be running at the same time)

Additional Inherited Members

14.79.1 Detailed Description

Derived application interface class which spawns simulation codes using fork/execvp/waitpid.

ForkApplicInterface is used on Unix systems and is a peer to SpawnApplicInterface for Windows systems.

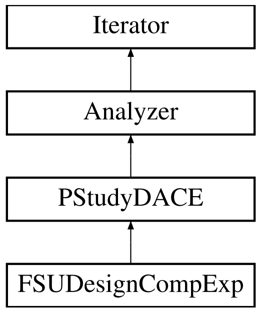
The documentation for this class was generated from the following files:

- ForkApplicInterface.hpp
- ForkApplicInterface.cpp

14.80 FSUDesignCompExp Class Reference

Wrapper class for the FSUDace QMC/CVT library.

Inheritance diagram for FSUDesignCompExp:



Public Member Functions

- FSUDesignCompExp (ProblemDescDB &problem_db, Model &model)

  primary constructor for building a standard DACE iterator
- FSUDesignCompExp (Model &model, int samples, int seed, unsigned short sampling_method)

  alternate constructor for building a DACE iterator on-the-fly
- ∼FSUDesignCompExp ()

  destructor
- bool resize ()

  reinitializes iterator based on new variable size

Protected Member Functions

- void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()

  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void post_input ()

  read tabular data for post-run mode
- void post_run (std::ostream &s)

  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- size_t num_samples () const
- void sampling_reset (size_t min_samples, bool all_data_flag, bool stats_flag)

  reset sampling iterator to use at least min_samples
- unsigned short sampling_scheme () const

  return sampling name
- void vary_pattern (bool pattern_flag)

  sets varyPattern in derived classes that support it
- void get_parameter_sets (Model &model)

  Generate one block of numSamples samples (ndim $*$ num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.
- void get_parameter_sets (Model &model, const size_t num_samples, RealMatrix &design_matrix)

  Generate one block of numSamples samples (ndim $*$ num_samples), populating design_matrix.

Private Member Functions

- void enforce_input_rules ()

    enforce sanity checks/modifications for the user input specification

Private Attributes

- int samplesSpec

    initial specification of number of samples
- size_t numSamples

    current number of samples to be evaluated
- bool allDataFlag

    flag which triggers the update of allVars/allResponses for use by Iterator::all_variables() and Iterator::all_responses()
- size_t numDACERuns

    counter for number of executions for this object
- bool latinizeFlag

    flag which specifies latinization of QMC or CVT sample sets
- IntVector sequenceStart

    Integer vector defining a starting index into the sequence for random variable sampled. Default is 0 0 0 (e.g. for three random variables).
- IntVector sequenceLeap

    Integer vector defining the leap number for each sequence being generated. Default is 1 1 1 (e.g. for three random vars.)
- IntVector primeBase

    Integer vector defining the prime base for each sequence being generated. Default is 2 3 5 (e.g., for three random vars.)
- int seedSpec

    the user seed specification for the random number generator (allows repeatable results)
- int randomSeed

    current seed for the random number generator
- bool varyPattern

    flag for continuing the random number or QMC sequence from a previous execution (e.g., for surrogate-based optimization) so that multiple executions are repeatable but not identical.
- int numCVTTrials

    specifies the number of sample points taken at internal CVT iteration
- int trialType

    Trial type in CVT. Specifies where the points are placed for consideration relative to the centroids. Choices are grid (2), halton (1), uniform (0), or random (-1). Default is random.

Additional Inherited Members

14.80.1 Detailed Description

Wrapper class for the FSUDace QMC/CVT library.

The FSUDesignCompExp class provides a wrapper for FSUDace, a C++ design of experiments library from Florida State University. This class uses quasi Monte Carlo (QMC) and Centroidal Voronoi Tesselation (CVT) methods to uniformly sample the parameter space spanned by the active bounds of the current Model. It returns all generated samples and their corresponding responses as well as the best sample found.

14.80.2 Constructor & Destructor Documentation

14.80.2.1 FSUDesignCompExp (ProblemDescDB & *problem_db,* Model & *model*)

primary constructor for building a standard DACE iterator

This constructor is called for a standard iterator built with data from probDescDB.

References Dakota::abort_handler(), ProblemDescDB::get_bool(), ProblemDescDB::get_int(), ProblemDescDB::get_iv(), ProblemDescDB::get_string(), Iterator::maxEvalConcurrency, Iterator::methodName, Analyzer::numContinuousVars, FSUDesignCompExp::numCVTTrials, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, FSUDesignCompExp::numSamples, FSUDesignCompExp::primeBase, Iterator::probDescDB, FSUDesignCompExp::randomSeed, FSUDesignCompExp::seedSpec, FSUDesignCompExp::sequenceLeap, FSUDesignCompExp::sequenceStart, FSUDesignCompExp::trialType, and FSUDesignCompExp::varyPattern.

14.80.2.2 FSUDesignCompExp (Model & *model,* int *samples,* int *seed,* unsigned short *sampling_method*)

alternate constructor for building a DACE iterator on-the-fly

This alternate constructor is used for instantiations on-the-fly, using only the incoming data. No problem description database queries are used.

References Dakota::abort_handler(), Iterator::maxEvalConcurrency, Iterator::methodName, Analyzer::numContinuousVars, FSUDesignCompExp::numCVTTrials, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, FSUDesignCompExp::numSamples, FSUDesignCompExp::primeBase, FSUDesignCompExp::randomSeed, FSUDesignCompExp::seedSpec, FSUDesignCompExp::sequenceLeap, FSUDesignCompExp::sequenceStart, and FSUDesignCompExp::trialType.

14.80.3 Member Function Documentation

14.80.3.1 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

References FSUDesignCompExp::enforce_input_rules(), FSUDesignCompExp::get_parameter_sets(), Analyzer::get_vbd_parameter_sets(), Iterator::iteratedModel, FSUDesignCompExp::numSamples, Analyzer::pre_run(), and PStudyDACE::varBasedDecompFlag.

14.80.3.2 void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References FSUDesignCompExp::allDataFlag, Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, Analyzer::numLSqTerms, Analyzer::numObjFns, and Iterator::subIteratorFlag.

14.80.3.3 void post_run (std::ostream & *s*) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Analyzer.

References Analyzer::allResponses, Analyzer::allSamples, SensAnalysisGlobal::compute_correlations(), Analyzer-::compute_vbd_stats(), FSUDesignCompExp::enforce_input_rules(), FSUDesignCompExp::numSamples, Analyzer::post_run(), PStudyDACE::pStudyDACESensGlobal, Iterator::subIteratorFlag, and PStudyDACE::var-BasedDecompFlag.

14.80.3.4 size_t num_samples ( ) const [inline], [protected], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.

References FSUDesignCompExp::numSamples.

Referenced by FSUDesignCompExp::get_parameter_sets().

14.80.3.5 void enforce_input_rules ( ) [private]

enforce sanity checks/modifications for the user input specification

Users may input a variety of quantities, but this function must enforce any restrictions imposed by the sampling algorithms.

References Dakota::abort_handler(), Iterator::methodName, Analyzer::numContinuousVars, FSUDesignCompExp-::numSamples, and FSUDesignCompExp::primeBase.

Referenced by FSUDesignCompExp::post_input(), FSUDesignCompExp::post_run(), and FSUDesignCompExp-::pre_run().

The documentation for this class was generated from the following files:

- FSUDesignCompExp.hpp
- FSUDesignCompExp.cpp

14.81 FunctionEvalFailure Class Reference

exception class for function evaluation failures

Inherits runtime_error.

Public Member Functions

- **FunctionEvalFailure** (const std::string &msg)

14.81.1 Detailed Description

exception class for function evaluation failures

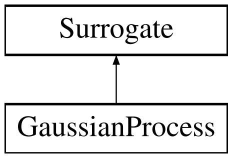
The documentation for this class was generated from the following file:

- dakota_global_defs.hpp

14.82 GaussianProcess Class Reference

The GaussianProcess constructs a Gaussian Process regressor surrogate given a matrix of data.

Inheritance diagram for GaussianProcess:



Public Member Functions

- GaussianProcess ()

  Constructor that uses defaultConfigOptions and does not build.
- GaussianProcess (const ParameterList &param_list)

  Constructor that sets configOptions but does not build.
- GaussianProcess (const std::string &param_list_yaml_filename)

  Constructor for the GaussianProcess that sets configOptions but does not build the GP.
- GaussianProcess (const MatrixXd &samples, const MatrixXd &response, const ParameterList &param_list)

  Constructor for the GaussianProcess that sets configOptions and builds the GP.
- GaussianProcess (const MatrixXd &samples, const MatrixXd &response, const std::string &param_list_yaml-_filename)

  Constructor for the GaussianProcess that sets configOptions and builds the GP.
- ∼GaussianProcess ()

  Default destructor.
- void build (const MatrixXd &eval_points, const MatrixXd &response) override

  Build the GP using specified build data.
- VectorXd value (const MatrixXd &eval_points, const int qoi) override

  Evaluate the Gaussian Process at a set of prediction points for a single qoi.
- VectorXd value (const MatrixXd &eval_points)

  Evaluate the Gaussian Process at a set of prediction points for QoI index 0.
- MatrixXd gradient (const MatrixXd &eval_points, const int qoi) override

  Evaluate the gradient of the Gaussian process at a set of prediction points for a single QoI.
- MatrixXd gradient (const MatrixXd &eval_points)

  Evaluate the gradient of the Gaussian process at a set of prediction points for QoI index 0.
- MatrixXd hessian (const MatrixXd &eval_point, const int qoi) override

  Evaluate the Hessian of the Gaussian process at a single point for a single QoI.
- MatrixXd hessian (const MatrixXd &eval_point)

  Evaluate the Hessian of the Gaussian process at a single point for QoI index 0.
- MatrixXd covariance (const MatrixXd &eval_points, const int qoi)

  Evaluate the covariance matrix for the Gaussian Process at a set of prediction points for a single QoI index.
- MatrixXd covariance (const MatrixXd &eval_points)

  Evaluate the covariance matrix for the Gaussian Process at a set of prediction points for QoI index 0.
- VectorXd variance (const MatrixXd &eval_points, const int qoi)

  Evaluate the variance of the Gaussian Process at a set of prediction points for a given QoI index.
- VectorXd variance (const MatrixXd &eval_points)

Evaluate the variance of the Gaussian Process at a set of prediction points for QoI index 0.

- void negative_marginal_log_likelihood (bool compute_grad, bool compute_gram, double &obj_value, VectorXd &obj_gradient)

  Evaluate the negative marginal loglikelihood and its gradient.
- void setup_hyperparameter_bounds (VectorXd &sigma_bounds, MatrixXd &length_scale_bounds, VectorXd &nugget_bounds)

  Initialize the hyperparameter bounds for MLE from values in configOptions.
- int get_num_opt_variables ()

  Get the number of optimization variables.
- int get_num_variables () const

  Get the dimension of the feature space.
- VectorXd get_objective_function_history ()

  Get the history of objective function values from MLE with restarts.
- MatrixXd get_objective_gradient_history ()

  Get the history of objective function gradients from MLE with restarts.
- MatrixXd get_theta_history ()

  Get the history of hyperparameter values from MLE with restarts.
- void set_opt_params (const std::vector< double > &opt_params)

  Update the vector of optimization parameters.
- std::shared_ptr< Surrogate > clone () const override

  clone derived Surrogate class for use in cross-validation

Private Member Functions

- void default_options () override

  Construct and populate the defaultConfigOptions.
- void compute_build_dists ()

  Compute squared distances between the scaled build points.
- void compute_pred_dists (const MatrixXd &scaled_pred_pts)

  Compute distances between build and prediction points. This includes build-prediction and prediction-prediction distance matrices.
- void compute_gram (const std::vector< MatrixXd > &dists2, bool add_nugget, bool compute_derivs, MatrixXd &gram)

  Compute a Gram matrix given a vector of squared distances and optionally compute its derivatives and/or adds nugget terms.
- void generate_initial_guesses (const VectorXd &sigma_bounds, const MatrixXd &length_scale_bounds, const VectorXd &nugget_bounds, const int num_restarts, const int seed, MatrixXd &initial_guesses)

  Randomly generate initial guesses for the optimization routine.
- void setup_default_optimization_params (Teuchos::RCP< ParameterList > rol_params)

  Set the default optimization parameters for ROL for GP hyperparameter estimation.
- template<class Archive >
  void serialize (Archive &archive, const unsigned int version)

  Serializer for save/load.

Private Attributes

- double fixedNuggetValue

  Small constant added to the diagonal of the Gram matrix to avoid ill-conditioning.
- MatrixXd eyeMatrix

  Identity matrix for the build points space.
- MatrixXd basisMatrix

Basis matrix for the sample points in polynomial regression.

- MatrixXd targetValues

  Target values for the surrogate dataset.
- MatrixXd scaledBuildPoints

  The scaled build points for the surrogate dataset.
- VectorXd thetaValues

  Vector of log-space hyperparameters.
- VectorXd betaValues

  Vector of polynomial coefficients.
- double estimatedNuggetValue

  Estimated nugget term.
- VectorXd bestThetaValues

  Vector of best hyperparameters from MLE with restarts.
- VectorXd bestBetaValues

  Vector of best polynomial coefficients from MLE with restarts.
- double bestEstimatedNuggetValue

  Best estimated nugget value from MLE with restarts.
- VectorXd objectiveFunctionHistory

  Final objective function values for each optimization run.
- MatrixXd objectiveGradientHistory

  Final objective function gradients for each optimization run.
- MatrixXd thetaHistory

  Final hyperparameter values for each optimization run.
- MatrixXd GramMatrix

  Gram matrix for the build points.
- VectorXd trendTargetResidual

  Difference between target values and trend predictions.
- VectorXd GramResidualSolution

  Cholesky solve for Gram matrix with trendTargetResidual rhs.
- std::vector< MatrixXd > GramMatrixDerivs

  Derivatives of the Gram matrix w.r.t. the hyperparameters.
- std::vector< MatrixXd > cwiseDists2

  Squared component-wise distances between points in the surrogate dataset.
- std::vector< MatrixXd > cwiseMixedDists

  Component-wise distances between prediction and build points.
- std::vector< MatrixXd > cwiseMixedDists2

  Squared component-wise distances between prediction and build points.
- std::vector< MatrixXd > cwisePredDists2

  Component-wise distances between prediction points.
- Eigen::LDLT< MatrixXd > CholFact

  Pivoted Cholesky factorization.
- bool hasBestCholFact

  Flag for recomputation of the best Cholesky factorization.
- MatrixXd predGramMatrix

  Gram matrix for the prediction points.
- MatrixXd predMixedGramMatrix

  Gram matrix for the mixed prediction/build points.
- MatrixXd predCovariance

  Covariance matrix for the prediction points.
- MatrixXd predBasisMatrix

  Polynomial basis matrix for the prediction points.

- std::shared_ptr
  < PolynomialRegression > polyRegression

  PolynomialRegression for trend function.
- std::string kernel_type

  Kernel type.
- std::shared_ptr< Kernel > kernel

  Kernel.
- const double betaBound = 1.0e20

  Large constant for polynomial coefficients upper/lower bounds.
- bool estimateTrend

  Bool for polynomial trend (i.e. semi-parametric GP) estimation.
- int numPolyTerms = 0

  Number of terms in polynomial trend.
- int numNuggetTerms = 0

  Number of terms for the (estimated) nugget parameter.
- bool estimateNugget

  Bool for nugget estimation.
- int verbosity

  Verbosity level.
- double bestObjFunValue = std::numeric_limits<double>::max()

  Final objective function value.
- const double PI = 3.14159265358979323846

  Numerical constant – needed for negative marginal log-likelihood.

Friends

- class boost::serialization::access

  Allow serializers access to private class data.

Additional Inherited Members

14.82.1 Detailed Description

The GaussianProcess constructs a Gaussian Process regressor surrogate given a matrix of data.

The Gaussian Process (GP) uses an anisotropic squared exponential kernel with a constant multiplicative scaling factor. This yields a total of num_features + 1 kernel hyperparameters. These parameters are internally transformed to a log-space vector (theta) for optimization and evaluation of the GP. Polynomial trend and nugget estimation are optional.

The GP's parameters are determined through maximum likelihood estimation (MLE) via minimization of the negative marginal log-likelihood function. ROL's implementation of L-BFGS-B is used to solve the optimization problem, and the algorithm may be run from multiple random initial guesses to increase the chance of finding the global minimum.

Once the GP is constructed its mean, variance, and covariance matrix can be computed for a set of prediction points. Gradients and Hessians are available.

14.82.2 Constructor & Destructor Documentation

14.82.2.1 GaussianProcess (const ParameterList & *param_list*)

Constructor that sets configOptions but does not build.

Parameters

in	*param_list*	List that overrides entries in defaultConfigOptions.

References Surrogate::configOptions, GaussianProcess::default_options(), and Surrogate::defaultConfigOptions.

14.82.2.2 GaussianProcess (const std::string & *param_list_yaml_filename*)

Constructor for the GaussianProcess that sets configOptions but does not build the GP.

Parameters

in	*param_list_yaml-_filename*	A ParameterList file (relative to the location of the Dakota input file) that overrides entries in defaultConfigOptions.

References Surrogate::configOptions, GaussianProcess::default_options(), and Surrogate::defaultConfigOptions.

14.82.2.3 GaussianProcess (const MatrixXd & *samples,* const MatrixXd & *response,* const ParameterList & *param_list*)

Constructor for the GaussianProcess that sets configOptions and builds the GP.

Parameters

in	*samples*	Matrix of data for surrogate construction - (num_samples by num_features)
in	*response*	Vector of targets for surrogate construction - (num_samples by num_qoi = 1; only 1 response is supported currently).
in	*param_list*	List that overrides entries in defaultConfigOptions

References GaussianProcess::build(), Surrogate::configOptions, and GaussianProcess::default_options().

14.82.2.4 GaussianProcess (const MatrixXd & *samples,* const MatrixXd & *response,* const std::string & *param_list_yaml_filename*)

Constructor for the GaussianProcess that sets configOptions and builds the GP.

Parameters

in	*samples*	Matrix of data for surrogate construction - (num_samples by num_features)
in	*response*	Vector of targets for surrogate construction - (num_samples by num_qoi = 1; only 1 response is supported currently).
in	*param_list_yaml-_filename*	A ParameterList file (relative to the location of the Dakota input file) that overrides entries in defaultConfigOptions.

References GaussianProcess::build(), Surrogate::configOptions, and GaussianProcess::default_options().

14.82.3 Member Function Documentation

14.82.3.1 void build (const MatrixXd & *eval_points,* const MatrixXd & *response*) [override], [virtual]

Build the GP using specified build data.

Parameters

in	*eval_points*	Matrix of data for surrogate construction - (num_samples by num_features)
in	*response*	Vector of targets for surrogate construction - (num_samples by num_qoi = 1; only 1 response is supported currently).

Implements Surrogate.

References GaussianProcess::basisMatrix, GaussianProcess::bestBetaValues, GaussianProcess::bestEstimatedNuggetValue, GaussianProcess::bestObjFunValue, GaussianProcess::bestThetaValues, GaussianProcess::betaBound, GaussianProcess::betaValues, GaussianProcess::CholFact, GaussianProcess::compute_build_dists(), GaussianProcess::compute_gram(), Surrogate::configOptions, GaussianProcess::cwiseDists2, Surrogate::dataScaler, Surrogate::defaultConfigOptions, GaussianProcess::estimatedNuggetValue, GaussianProcess::estimateNugget, GaussianProcess::estimateTrend, GaussianProcess::eyeMatrix, GaussianProcess::fixedNuggetValue, GaussianProcess::generate_initial_guesses(), GaussianProcess::GramMatrix, GaussianProcess::GramMatrixDerivs, GaussianProcess::hasBestCholFact, GaussianProcess::kernel, dakota::surrogates::kernel_factory(), GaussianProcess::kernel_type, GaussianProcess::negative_marginal_log_likelihood(), GaussianProcess::numNuggetTerms, GaussianProcess::numPolyTerms, Surrogate::numQOI, Surrogate::numSamples, Surrogate::numVariables, GaussianProcess::objectiveFunctionHistory, GaussianProcess::objectiveGradientHistory, GaussianProcess::polyRegression, Surrogate::responseOffset, Surrogate::responseScaleFactor, DataScaler::scale_samples(), GaussianProcess::scaledBuildPoints, dakota::util::scaler_factory(), DataScaler::scaler_type(), GaussianProcess::setup_default_optimization_params(), GaussianProcess::setup_hyperparameter_bounds(), GaussianProcess::targetValues, GaussianProcess::thetaHistory, GaussianProcess::thetaValues, and GaussianProcess::verbosity.

Referenced by GaussianProcess::GaussianProcess().

14.82.3.2 VectorXd value (const MatrixXd & *eval_points,* const int *qoi*) [override], [virtual]

Evaluate the Gaussian Process at a set of prediction points for a single qoi.

Parameters

in	*eval_points*	Matrix for prediction points - (num_points by num_features).
in	*qoi*	Index for surrogate QoI.

Returns

Mean of the Gaussian process at the prediction points.

Implements Surrogate.

References GaussianProcess::basisMatrix, GaussianProcess::betaValues, GaussianProcess::CholFact, GaussianProcess::compute_gram(), GaussianProcess::compute_pred_dists(), GaussianProcess::cwiseDists2, GaussianProcess::cwiseMixedDists2, Surrogate::dataScaler, GaussianProcess::estimateTrend, GaussianProcess::GramMatrix, GaussianProcess::hasBestCholFact, Surrogate::numVariables, GaussianProcess::polyRegression, GaussianProcess::predBasisMatrix, GaussianProcess::predMixedGramMatrix, Surrogate::responseOffset, Surrogate::responseScaleFactor, DataScaler::scale_samples(), dakota::silence_unused_args(), and GaussianProcess::targetValues.

14.82.3.3 VectorXd value (const MatrixXd & *eval_points*) [inline]

Evaluate the Gaussian Process at a set of prediction points for QoI index 0.

Parameters

in	*eval_points*	Matrix for prediction points - (num_points by num_features).

Returns

Mean of the Gaussian process at the prediction points.

References Surrogate::value().

14.82.3.4 MatrixXd gradient (const MatrixXd & *eval_points,* const int *qoi*) [override], [virtual]

Evaluate the gradient of the Gaussian process at a set of prediction points for a single QoI.

Parameters

in	*eval_points*	Coordinates of the prediction points - (num_pts by num_features).
in	*qoi*	Index of response/QoI for which to compute derivatives.

Returns

Matrix of gradient vectors at the prediction points - (num_pts by num_features).

Reimplemented from Surrogate.

References GaussianProcess::basisMatrix, GaussianProcess::betaValues, GaussianProcess::CholFact, GaussianProcess::compute_gram(), GaussianProcess::compute_pred_dists(), GaussianProcess::cwiseDists2, GaussianProcess::cwiseMixedDists, GaussianProcess::cwiseMixedDists2, Surrogate::dataScaler, GaussianProcess::estimateTrend, GaussianProcess::GramMatrix, GaussianProcess::hasBestCholFact, GaussianProcess::kernel, Surrogate::numVariables, GaussianProcess::polyRegression, GaussianProcess::predMixedGramMatrix, Surrogate::responseScaleFactor, DataScaler::scale_samples(), dakota::silence_unused_args(), GaussianProcess::targetValues, and GaussianProcess::thetaValues.

14.82.3.5 MatrixXd gradient (const MatrixXd & *eval_points*) [inline]

Evaluate the gradient of the Gaussian process at a set of prediction points for QoI index 0.

Parameters

in	*eval_points*	Coordinates of the prediction points - (num_pts by num_features).

Returns

Matrix of gradient vectors at the prediction points - (num_pts by num_features).

References Surrogate::gradient().

14.82.3.6 MatrixXd hessian (const MatrixXd & *eval_point,* const int *qoi*) [override], [virtual]

Evaluate the Hessian of the Gaussian process at a single point for a single QoI.

Parameters

in	*eval_point*	Coordinates of the prediction point - (1 by num_features).
in	*qoi*	Index of response/QoI for which to compute derivatives

Returns

Hessian matrix at the prediction point - (num_features by num_features).

Reimplemented from Surrogate.

References GaussianProcess::basisMatrix, GaussianProcess::betaValues, GaussianProcess::CholFact, GaussianProcess::compute_gram(), GaussianProcess::compute_pred_dists(), GaussianProcess::cwiseDists2, GaussianProcess::cwiseMixedDists, GaussianProcess::cwiseMixedDists2, Surrogate::dataScaler, GaussianProcess::estimateTrend, GaussianProcess::GramMatrix, GaussianProcess::hasBestCholFact, GaussianProcess::kernel, Surrogate::numVariables, GaussianProcess::polyRegression, GaussianProcess::predMixedGramMatrix, Surrogate::responseScaleFactor, DataScaler::scale_samples(), dakota::silence_unused_args(), GaussianProcess::targetValues, and GaussianProcess::thetaValues.

14.82.3.7 MatrixXd hessian (const MatrixXd & *eval_point*) [inline]

Evaluate the Hessian of the Gaussian process at a single point for QoI index 0.

Parameters

in	*eval_point*	Coordinates of the prediction point - (1 by num_features).

Returns

Hessian matrix at the prediction point - (num_features by num_features).

References Surrogate::hessian().

14.82.3.8 MatrixXd covariance (const MatrixXd & *eval_points*, const int *qoi*)

Evaluate the covariance matrix for the Gaussian Process at a set of prediction points for a single QoI index.

Parameters

in	*eval_points*	Matrix for the prediction points - (num_points by num_features).
in	*qoi*	Index of response/QoI for which to compute derivatives

Returns

[out] Covariance matrix for the Gaussian process at the prediction points.

References GaussianProcess::basisMatrix, GaussianProcess::betaValues, GaussianProcess::CholFact, GaussianProcess::compute_gram(), GaussianProcess::compute_pred_dists(), GaussianProcess::cwiseDists2, GaussianProcess::cwiseMixedDists2, GaussianProcess::cwisePredDists2, Surrogate::dataScaler, GaussianProcess::estimateTrend, GaussianProcess::GramMatrix, GaussianProcess::hasBestCholFact, Surrogate::numVariables, GaussianProcess::polyRegression, GaussianProcess::predBasisMatrix, GaussianProcess::predCovariance, GaussianProcess::predGramMatrix, GaussianProcess::predMixedGramMatrix, Surrogate::responseScaleFactor, DataScaler::scale_samples(), dakota::silence_unused_args(), and GaussianProcess::targetValues.

Referenced by GaussianProcess::covariance(), and GaussianProcess::variance().

14.82.3.9 MatrixXd covariance (const MatrixXd & *eval_points*) [inline]

Evaluate the covariance matrix for the Gaussian Process at a set of prediction points for QoI index 0.

Parameters

in	*eval_points*	Matrix for the prediction points - (num_points by num_features).

Returns

[out] Covariance of the Gaussian process at the prediction points.

References GaussianProcess::covariance().

14.82.3.10 VectorXd variance (const MatrixXd & *eval_points*, const int *qoi*)

Evaluate the variance of the Gaussian Process at a set of prediction points for a given QoI index.

Parameters

in	*eval_points*	Matrix for the prediction points - (num_points by num_features).

in	*qoi*	Index of response/QoI for which to compute derivatives

Returns

[out] Variance of the Gaussian process at the prediction points.

References GaussianProcess::covariance(), and dakota::silence_unused_args().

Referenced by SurrogatesGPApprox::prediction_variance(), PYBIND11_MODULE(), and GaussianProcess::variance().

14.82.3.11 VectorXd variance (const MatrixXd & *eval_points*) [inline]

Evaluate the variance of the Gaussian Process at a set of prediction points for QoI index 0.

Parameters

in	*eval_points*	Matrix for the prediction points - (num_points by num_features).

Returns

[out] Variance of the Gaussian process at the prediction points.

References GaussianProcess::variance().

14.82.3.12 void negative_marginal_log_likelihood (bool *compute_grad,* bool *compute_gram,* double & *obj_value,* VectorXd & *obj_gradient*)

Evaluate the negative marginal loglikelihood and its gradient.

Parameters

in	*compute_grad*	Flag for computation of gradient.
in	*compute_gram*	Flag for various Gram matrix calculations.
out	*obj_value*	Value of the objection function.
out	*obj_gradient*	Gradient of the objective function.

References GaussianProcess::basisMatrix, GaussianProcess::betaValues, GaussianProcess::CholFact, GaussianProcess::compute_gram(), GaussianProcess::cwiseDists2, GaussianProcess::estimatedNuggetValue, GaussianProcess::estimateNugget, GaussianProcess::estimateTrend, GaussianProcess::eyeMatrix, GaussianProcess::GramMatrix, GaussianProcess::GramMatrixDerivs, GaussianProcess::GramResidualSolution, GaussianProcess::numPolyTerms, Surrogate::numSamples, Surrogate::numVariables, GaussianProcess::PI, GaussianProcess::targetValues, and GaussianProcess::trendTargetResidual.

Referenced by GaussianProcess::build(), GP_Objective::gradient(), and GP_Objective::value().

14.82.3.13 void setup_hyperparameter_bounds (VectorXd & *sigma_bounds,* MatrixXd & *length_scale_bounds,* VectorXd & *nugget_bounds*)

Initialize the hyperparameter bounds for MLE from values in configOptions.

Parameters

out	*sigma_bounds*	Bounds for the sigma (i.e. scale) hyperparameter.
out	*length_scale_bounds*	Bounds for the anisotropic length-scale hyperparameters.

out	*nugget_bounds*	Bounds for the estimated nugget hyperparameter.

References Surrogate::configOptions, GaussianProcess::estimateNugget, GaussianProcess::numNuggetTerms, and Surrogate::numVariables.

Referenced by GaussianProcess::build().

14.82.3.14 int get_num_opt_variables ( )

Get the number of optimization variables.

Returns

Number of total optimization variables (hyperparameters + trend coefficients + nugget)

References GaussianProcess::numNuggetTerms, GaussianProcess::numPolyTerms, and Surrogate::numVariables.

Referenced by GP_Objective::GP_Objective().

14.82.3.15 int get_num_variables ( ) const

Get the dimension of the feature space.

Returns

numVariables The dimension of the feature space.

References Surrogate::numVariables.

14.82.3.16 VectorXd get_objective_function_history ( ) [inline]

Get the history of objective function values from MLE with restarts.

Returns

objectiveFunctionHistory Vector of final objective function values.

References GaussianProcess::objectiveFunctionHistory.

14.82.3.17 MatrixXd get_objective_gradient_history ( ) [inline]

Get the history of objective function gradients from MLE with restarts.

Returns

objectiveGradientHistory Matrix of final objective funciton values

- (num_restarts, num_hyperparameters).

References GaussianProcess::objectiveGradientHistory.

14.82.3.18 MatrixXd get_theta_history ( ) [inline]

Get the history of hyperparameter values from MLE with restarts.

Returns

thetaHistory Vector of final hyperparameter (theta) values

- (num_restarts, num_hyperparameters).

References GaussianProcess::thetaHistory.

Referenced by PYBIND11_MODULE().

14.82.3.19 void set_opt_params (const std::vector< double > & *opt_params*)

Update the vector of optimization parameters.

Parameters

in	*opt_params*	Vector of optimization parameter values.

References GaussianProcess::betaValues, GaussianProcess::estimatedNuggetValue, GaussianProcess::estimateNugget, GaussianProcess::estimateTrend, GaussianProcess::numPolyTerms, Surrogate::numVariables, and GaussianProcess::thetaValues.

Referenced by GP_Objective::gradient(), and GP_Objective::value().

14.82.3.20 void compute_pred_dists (const MatrixXd & *scaled_pred_pts*) [private]

Compute distances between build and prediction points. This includes build-prediction and prediction-prediction distance matrices.

Parameters

in	*scaled_pred_pts*	Matrix of scaled prediction points.

References GaussianProcess::cwiseMixedDists, GaussianProcess::cwiseMixedDists2, GaussianProcess::cwisePredDists2, Surrogate::numSamples, Surrogate::numVariables, and GaussianProcess::scaledBuildPoints.

Referenced by GaussianProcess::covariance(), GaussianProcess::gradient(), GaussianProcess::hessian(), and GaussianProcess::value().

14.82.3.21 void compute_gram (const std::vector< MatrixXd > & *dists2,* bool *add_nugget,* bool *compute_derivs,* MatrixXd & *gram*) [private]

Compute a Gram matrix given a vector of squared distances and optionally compute its derivatives and/or adds nugget terms.

Parameters

in	*dists2*	Vector of squared distance matrices.
in	*add_nugget*	Bool for whether or add nugget terms.
in	*compute_derivs*	Bool for whether or not to compute the derivatives of the Gram matrix.
out	*gram*	Gram matrix.

References GaussianProcess::estimatedNuggetValue, GaussianProcess::estimateNugget, GaussianProcess::fixedNuggetValue, GaussianProcess::GramMatrixDerivs, GaussianProcess::kernel, and GaussianProcess::thetaValues.

Referenced by GaussianProcess::build(), GaussianProcess::covariance(), GaussianProcess::gradient(), GaussianProcess::hessian(), GaussianProcess::negative_marginal_log_likelihood(), and GaussianProcess::value().

14.82.3.22 void generate_initial_guesses (const VectorXd & *sigma_bounds*, const MatrixXd & *length_scale_bounds*, const VectorXd & *nugget_bounds*, const int *num_restarts*, const int *seed*, MatrixXd & *initial_guesses*) [private]

Randomly generate initial guesses for the optimization routine.

Parameters

in	*sigma_bounds*	Bounds for the scaling hyperparameter (sigma).
in	*length_scale_-bounds*	Bounds for the length scales for each feature (l).
in	*nugget_bounds*	Bounds for the nugget term.
in	*num_restarts*	Number of restarts for the optimizer.
in	*seed*	Seed for the random number generator.
out	*initial_guesses*	Matrix of initial guesses.

References dakota::util::create_uniform_random_double_matrix(), GaussianProcess::estimateNugget, Gaussian-Process::estimateTrend, GaussianProcess::numNuggetTerms, GaussianProcess::numPolyTerms, and Surrogate-::numVariables.

Referenced by GaussianProcess::build().

14.82.3.23 void setup_default_optimization_params (Teuchos::RCP< ParameterList > *rol_params*) [private]

Set the default optimization parameters for ROL for GP hyperparameter estimation.

Parameters

in	*rol_params*	RCP to a Teuchos::ParameterList of ROL's options.

Referenced by GaussianProcess::build().

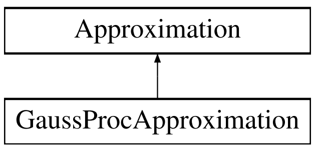
The documentation for this class was generated from the following files:

- SurrogatesGaussianProcess.hpp
- SurrogatesGaussianProcess.cpp

14.83 GaussProcApproximation Class Reference

Derived approximation class for Gaussian Process implementation.

Inheritance diagram for GaussProcApproximation:



Public Member Functions

- GaussProcApproximation ()

  default constructor
- GaussProcApproximation (const SharedApproxData &shared_data)

  alternate constructor
- GaussProcApproximation (const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

  standard constructor
- ∼GaussProcApproximation ()

  destructor

Protected Member Functions

- int min_coefficients () const

  return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- void build ()

  find the covariance parameters governing the Gaussian process response
- Real value (const Variables &vars)

  retrieve the function value for a given parameter set
- const RealVector & gradient (const Variables &vars)

  retrieve the function gradient at the predicted value for a given parameter set
- Real prediction_variance (const Variables &vars)

  retrieve the variance of the predicted value for a given parameter set

Private Member Functions

- void GPmodel_build ()

  Function to compute hyperparameters governing the GP.
- void GPmodel_apply (const RealVector &new_x, bool variance_flag, bool gradients_flag)

  Function returns a response value using the GP surface.
- void normalize_training_data ()

  Normalizes the initial inputs upon which the GP surface is based.
- void get_trend ()

  Gets the trend (basis) functions for the calculation of the mean of the GP If the order = 0, the trend is a constant, if the order = 1, trend is linear, if order = 2, trend is quadratic.
- void get_beta_coefficients ()

  Gets the beta coefficients for the calculation of the mean of the GP.
- int get_cholesky_factor ()

  Gets the Cholesky factorization of the covariance matrix, with error checking.
- void get_process_variance ()

  Gets the estimate of the process variance given the values of beta and the correlation lengthscales.
- void get_cov_matrix ()

  calculates the covariance matrix for a given set of input points
- void get_cov_vector ()

  calculates the covariance vector between a new point x and the set of inputs upon which the GP is based
- void optimize_theta_global ()

  sets up and performs the optimization of the negative log likelihood to determine the optimal values of the covariance parameters using NCSUDirect
- void optimize_theta_multipoint ()

  sets up and performs the optimization of the negative log likelihood to determine the optimal values of the covariance parameters using a gradient-based solver and multiple starting points
- void predict (bool variance_flag, bool gradients_flag)

  Calculates the predicted new response value for x in normalized space.
- Real calc_nll ()

  calculates the negative log likelihood function (based on covariance matrix)
- void calc_grad_nll ()

  Gets the gradient of the negative log likelihood function with respect to the correlation lengthscales, theta.
- void get_grad_cov_vector ()

  Calculate the derivatives of the covariance vector, with respect to each componeent of x.
- void run_point_selection ()

  Runs the point selection algorithm, which will choose a subset of the training set with which to construct the GP model, and estimate the necessary parameters.

- void initialize_point_selection ()

  Initializes the point selection routine by choosing a small initial subset of the training points.
- void pointsel_get_errors (RealArray &delta)

  Uses the current GP model to compute predictions at all of the training points and find the errors.
- int addpoint (int, IntArray &added_index)

  Adds a point to the effective training set. Returns 1 on success.
- int pointsel_add_sel (const RealArray &delta)

  Accepts a vector of unsorted prediction errors, determines which points should be added to the effective training set, and adds them.
- Real maxval (const RealArray &) const

  Return the maximum value of the elements in a vector.
- void pointsel_write_points ()

  Writes out the training set before and after point selection.
- void lhood_2d_grid_eval ()

  For problems with 2D input, evaluates the negative log likelihood on a grid.
- void writex (const char[])

  Writes out the current training set (in original units) to a specified file.
- void writeCovMat (char[])

  Writes out the covariance matrix to a specified file.

Static Private Member Functions

- static void negloglik (int mode, int n, const Teuchos::SerialDenseVector< int, double > &X, Real &fx, Teuchos::SerialDenseVector< int, double > &grad_x, int &result_mode)

  static function used by OPT++ as the objective function to optimize the hyperparameters in the covariance of the GP by minimizing the negative log likelihood
- static void constraint_eval (int mode, int n, const Teuchos::SerialDenseVector< int, double > &X, Teuchos::SerialDenseVector< int, double > &g, Teuchos::SerialDenseMatrix< int, double > &gradC, int &result_mode)

  static function used by OPT++ as the constraint function in the optimization of the negative log likelihood. Currently this function is empty: it is an unconstrained optimization.
- static double negloglikNCSU (const RealVector &x)

  function used by NCSUOptimizer to optimize negloglik objective

Private Attributes

- Real approxValue

  value of the approximation returned by value()
- Real approxVariance

  value of the approximation returned by prediction_variance()
- RealMatrix trainPoints

  A 2-D array (num sample sites = rows, num vars = columns) used to create the Gaussian process.
- RealMatrix trainValues

  An array of response values; one response value per sample site.
- RealVector trainMeans

  The mean of the input columns of trainPoints.
- RealVector trainStdvs

  The standard deviation of the input columns of trainPoints.
- RealMatrix normTrainPoints

  Current working set of normalized points upon which the GP is based.
- RealMatrix trendFunction

matrix to hold the trend function

- RealMatrix betaCoeffs

  matrix to hold the beta coefficients for the trend function
- RealSymMatrix covMatrix

  The covariance matrix where each element (i,j) is the covariance between points Xi and Xj in the initial set of samples.
- RealMatrix covVector

  The covariance vector where each element (j,0) is the covariance between a new point X and point Xj from the initial set of samples.
- RealMatrix approxPoint

  Point at which a prediction is requested. This is currently a single point, but it could be generalized to be a vector of points.
- RealMatrix gradNegLogLikTheta

  matrix to hold the gradient of the negative log likelihood with respect to the theta correlation terms
- Teuchos::SerialSpdDenseSolver
  $<$ int, Real $>$ covSlvr

  The global solver for all computations involving the inverse of the covariance matrix.
- RealMatrix gradCovVector

  A matrix, where each column is the derivative of the covVector with respect to a particular componenet of X.
- RealMatrix normTrainPointsAll

  Set of all original samples available.
- RealMatrix trainValuesAll

  All original samples available.
- RealMatrix trendFunctionAll

  Trend function values corresponding to all original samples.
- RealMatrix Rinv_YFb

  Matrix for storing inverse of correlation matrix Rinv∗(Y-FB)
- size_t numObs

  The number of observations on which the GP surface is built.
- size_t numObsAll

  The original number of observations.
- short trendOrder

  The number of variables in each X variable (number of dimensions of the problem).
- RealVector thetaParams

  Theta is the vector of covariance parameters for the GP. We determine the values of theta by optimization Currently, the covariance function is theta[0]∗exp(-0.5∗sume)+delta∗pow(sige,2). sume is the sum squared of weighted distances; it involves a sum of theta[1](Xi(1)-Xj(1))^2 + theta[2](Xi(2)-Xj(2))^2 + ... where Xi(1) is the first dimension value of multi-dimensional variable Xi. delta∗pow(sige,2) is a jitter term used to improve matrix computations. delta is zero for the covariance between different points and 1 for the covariance between the same point. sige is the underlying process error.
- Real procVar

  The process variance, the multiplier of the correlation matrix.
- IntArray pointsAddedIndex

  Used by the point selection algorithm, this vector keeps track all points which have been added.
- int cholFlag

  A global indicator for success of the Cholesky factorization.
- bool usePointSelection

  a flag to indicate the use of point selection

Static Private Attributes

- static GaussProcApproximation ∗ GPinstance

  pointer to the active object instance used within the static evaluator

Additional Inherited Members

14.83.1 Detailed Description

Derived approximation class for Gaussian Process implementation.

The GaussProcApproximation class provides a global approximation (surrogate) based on a Gaussian process. The Gaussian process is built after normalizing the function values, with zero mean. Opt++ is used to determine the optimal values of the covariance parameters, those which minimize the negative log likelihood function.

14.83.2 Constructor & Destructor Documentation

14.83.2.1 GaussProcApproximation ( ) [inline]

default constructor

alternate constructor used by EffGlobalOptimization and NonDGlobalReliability that does not use a problem database defaults here are no point selectinn and quadratic trend function.

14.83.3 Member Function Documentation

14.83.3.1 void GPmodel_apply (const RealVector & *new_x,* bool *variance_flag,* bool *gradients_flag*) [private]

Function returns a response value using the GP surface.

The response value is computed at the design point specified by the RealVector function argument.

References Dakota::abort_handler(), GaussProcApproximation::approxPoint, GaussProcApproximation::get_cov-_vector(), GaussProcApproximation::predict(), Approximation::sharedDataRep, GaussProcApproximation::train-Means, and GaussProcApproximation::trainStdvs.

Referenced by GaussProcApproximation::gradient(), GaussProcApproximation::pointsel_get_errors(), GaussProc-Approximation::prediction_variance(), and GaussProcApproximation::value().

14.83.4 Member Data Documentation

14.83.4.1 short trendOrder [private]

The number of variables in each X variable (number of dimensions of the problem).

The order of the basis function for the mean of the GP If the order = 0, the trend is a constant, if the order = 1, trend is linear, if order = 2, trend is quadratic.

Referenced by GaussProcApproximation::GaussProcApproximation(), GaussProcApproximation::get_beta_-coefficients(), GaussProcApproximation::get_trend(), GaussProcApproximation::GPmodel_build(), and Gauss-ProcApproximation::predict().

The documentation for this class was generated from the following files:

- GaussProcApproximation.hpp
- GaussProcApproximation.cpp

14.84 GeneralReader Class Reference

Utility used in derived read_core to read in generic format.

Public Member Functions

- template<typename ArrayType >
  void **operator()** (std::istream &s, size_t start_index, size_t num_items, ArrayType &array_data, StringMultiArrayView label_array)

14.84.1 Detailed Description

Utility used in derived read_core to read in generic format.

The documentation for this class was generated from the following file:

- DakotaVariables.hpp

14.85 GeneralWriter Class Reference

Utility used in derived write_core to write in generic format.

Public Member Functions

- template<typename ArrayType >
  void **operator()** (std::ostream &s, size_t start_index, size_t num_items, const ArrayType &array_data, StringMultiArrayConstView label_array)

14.85.1 Detailed Description

Utility used in derived write_core to write in generic format.

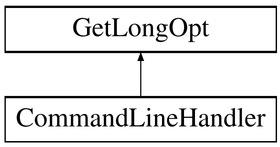
The documentation for this class was generated from the following file:

- DakotaVariables.hpp

14.86 GetLongOpt Class Reference

GetLongOpt is a general command line utility from S. Manoharan (Advanced Computer Research Institute, Lyon, France).

Inheritance diagram for GetLongOpt:



Public Types

- enum OptType { Valueless, OptionalValue, MandatoryValue }

  enum for different types of values associated with command line options.

Public Member Functions

- GetLongOpt (const char optmark= '-')
  Constructor.
- ∼GetLongOpt ()
  Destructor.
- int parse (int argc, char ∗const ∗argv)
  parse the command line args (argc, argv).
- int parse (char ∗const str, char ∗const p)
  parse a string of options (typically given from the environment).
- int enroll (const char ∗const opt, const OptType t, const char ∗const desc, const char ∗const val)
  Add an option to the list of valid command options.
- const char ∗ retrieve (const char ∗const opt) const
  Retrieve value of option.
- void usage (std::ostream &outfile=Cout) const
  Print usage information to outfile.
- void usage (const char ∗str)
  Change header of usage output to str.
- void store (const char ∗name, const char ∗value)
  Store a specified option value.

Private Member Functions

- char ∗ basename (char ∗const p) const
  extract the base name from a string as delimited by '/'
- int setcell (Cell ∗c, char ∗valtoken, char ∗nexttoken, const char ∗p)
  internal convenience function for setting Cell::value

Private Attributes

- Cell ∗ table
  option table
- const char ∗ ustring
  usage message
- char ∗ pname
  program basename
- char optmarker
  option marker
- int enroll_done
  finished enrolling
- Cell ∗ last
  last entry in option table

14.86.1 Detailed Description

GetLongOpt is a general command line utility from S. Manoharan (Advanced Computer Research Institute, Lyon, France).

GetLongOpt manages the definition and parsing of "long options." Command line options can be abbreviated as long as there is no ambiguity. If an option requires a value, the value should be separated from the option either by whitespace or an "=".

14.86.2 Member Enumeration Documentation

14.86.2.1 enum OptType

enum for different types of values associated with command line options.

Enumerator

Valueless option that may never have a value

OptionalValue option with optional value

MandatoryValue option with required value

14.86.3 Constructor & Destructor Documentation

14.86.3.1 GetLongOpt (const char *optmark* = ′ −′)

Constructor.

Constructor for GetLongOpt takes an optional argument: the option marker. If unspecified, this defaults to '-', the standard (?) Unix option marker.

References GetLongOpt::enroll_done, GetLongOpt::last, GetLongOpt::optmarker, GetLongOpt::table, and GetLongOpt::ustring.

14.86.4 Member Function Documentation

14.86.4.1 int parse (int *argc,* char ∗const ∗ *argv*)

parse the command line args (argc, argv).

A return value $<$ 1 represents a parse error. Appropriate error messages are printed when errors are seen. parse returns the the optind (see getopt(3)) if parsing is successful.

References GetLongOpt::basename(), GetLongOpt::enroll_done, GetLongOpt::optmarker, GetLongOpt::pname, GetLongOpt::setcell(), and GetLongOpt::table.

Referenced by CommandLineHandler::check_usage().

14.86.4.2 int parse (char ∗const *str,* char ∗const *p*)

parse a string of options (typically given from the environment).

A return value $<$ 1 represents a parse error. Appropriate error messages are printed when errors are seen. parse takes two strings: the first one is the string to be parsed and the second one is a string to be prefixed to the parse errors.

References GetLongOpt::enroll_done, GetLongOpt::optmarker, GetLongOpt::setcell(), and GetLongOpt::table.

14.86.4.3 int enroll (const char ∗const *opt,* const OptType *t,* const char ∗const *desc,* const char ∗const *val*)

Add an option to the list of valid command options.

enroll adds option specifications to its internal database. The first argument is the option sting. The second is an enum saying if the option is a flag (Valueless), if it requires a mandatory value (MandatoryValue) or if it takes an optional value (OptionalValue). The third argument is a string giving a brief description of the option. This description will be used by GetLongOpt::usage. GetLongOpt, for usage-printing, uses {$val} to represent values needed by the options. {$<$$val$>$} is a mandatory value and {[$val]} is an optional value. The final argument to enroll is the default string to be returned if the option is not specified. For flags (options with Valueless), use "" (empty string, or in fact any arbitrary string) for specifying TRUE and 0 (null pointer) to specify FALSE.

References GetLongOpt::enroll_done, GetLongOpt::last, and GetLongOpt::table.

Referenced by CommandLineHandler::initialize_options().

14.86.4.4 const char * retrieve (const char *const *opt*) const

Retrieve value of option.

The values of the options that are enrolled in the database can be retrieved using retrieve. This returns a string and this string should be converted to whatever type you want. See atoi, atof, atol, etc. If a "parse" is not done before retrieving all you will get are the default values you gave while enrolling! Ambiguities while retrieving (may happen when options are abbreviated) are resolved by taking the matching option that was enrolled last. For example, -{v} will expand to {-verify}. If you try to retrieve something you didn't enroll, you will get a warning message.

References GetLongOpt::optmarker, and GetLongOpt::table.

Referenced by CommandLineHandler::check_usage(), ProgramOptions::manage_run_modes(), ProgramOptions::ProgramOptions(), and CommandLineHandler::read_restart_evals().

14.86.4.5 void usage (const char * *str*) [inline]

Change header of usage output to str.

GetLongOpt::usage is overloaded. If passed a string "str", it sets the internal usage string to "str". Otherwise it simply prints the command usage.

References GetLongOpt::ustring.

The documentation for this class was generated from the following files:

- CommandLineHandler.hpp
- CommandLineHandler.cpp

14.87 GP_Objective Class Reference

ROL objective function for the Gaussian Process (GP) surrogate.

Inherits Objective< double >.

Public Member Functions

- GP_Objective (GaussianProcess &gp_model)

    Constructor for GP_Objective.
- double value (const ROL::Vector< double > &p, double &tol)

    Get the value of the objective function at a point.
- void gradient (ROL::Vector< double > &g, const ROL::Vector< double > &p, double &tol)

    Get the gradient of the objective function at a point.

Private Member Functions

- bool pdiff (const std::vector< double > &pnew)

    Compute the l2 norm of the difference between new and old parameter vectors.
- ROL::Ptr< const std::vector
< double > > getVector (const ROL::Vector< double > &vec)

    Convert a const ROL Vector to a ROL::Ptr<const std::vector>
- ROL::Ptr< std::vector< double > > getVector (ROL::Vector< double > &vec)

    Convert a ROL Vector to a ROL::Ptr<std::vector>

Private Attributes

- GaussianProcess & gp

  Pointer to the GaussianProcess surrogate.
- int nopt

  Number of optimization variables.
- double Jold

  Previously computed value of the objective function.
- VectorXd grad_old

  Previously computed gradient of the objective function.
- VectorXd pold

  Previous value of the parameter vector.

14.87.1 Detailed Description

ROL objective function for the Gaussian Process (GP) surrogate.

14.87.2 Constructor & Destructor Documentation

14.87.2.1 GP_Objective (GaussianProcess & *gp_model*)

Constructor for GP_Objective.

Parameters

in	*gp_model*	Reference to the GaussianProcess surrogate.

References GaussianProcess::get_num_opt_variables(), GP_Objective::gp, GP_Objective::grad_old, GP_-Objective::Jold, GP_Objective::nopt, and GP_Objective::pold.

14.87.3 Member Function Documentation

14.87.3.1 double value (const ROL::Vector< double > & *p*, double & *tol*)

Get the value of the objective function at a point.

Parameters

in	*p*	ROL vector of parameters.
in	*tol*	Tolerance for inexact evaluation (not used here).

References GP_Objective::getVector(), GP_Objective::gp, GaussianProcess::negative_marginal_log_likelihood(), GP_Objective::nopt, GP_Objective::pdiff(), GaussianProcess::set_opt_params(), and dakota::silence_unused_-args().

14.87.3.2 void gradient (ROL::Vector< double > & *g*, const ROL::Vector< double > & *p*, double & *tol*)

Get the gradient of the objective function at a point.

Parameters

out	*g*	Gradient of the objective function.

in	*p*	ROL vector of parameters.
in	*tol*	Tolerance for inexact evaluation (not used here).

References GP_Objective::getVector(), GP_Objective::gp, GaussianProcess::negative_marginal_log_likelihood(), GP_Objective::nopt, GP_Objective::pdiff(), GaussianProcess::set_opt_params(), and dakota::silence_unused_-args().

14.87.3.3 bool pdiff (const std::vector< double > & *pnew*) [private]

Compute the l2 norm of the difference between new and old parameter vectors.

Parameters

in	*pnew*	New value of the parameter vector.

References dakota::near_zero, GP_Objective::nopt, and GP_Objective::pold.

Referenced by GP_Objective::gradient(), and GP_Objective::value().

14.87.3.4 ROL::Ptr<const std::vector<double> > getVector (const ROL::Vector< double > & *vec*) [inline], [private]

Convert a const ROL Vector to a ROL::Ptr<const std::vector>

Parameters

in	*vec*	const ROL vector

Referenced by GP_Objective::getVector(), GP_Objective::gradient(), and GP_Objective::value().

14.87.3.5 ROL::Ptr<std::vector<double> > getVector (ROL::Vector< double > & *vec*) [inline], [private]

Convert a ROL Vector to a ROL::Ptr<std::vector>

Parameters

in	*vec*	ROL vector

References GP_Objective::getVector().

The documentation for this class was generated from the following files:

- SurrogatesGPObjective.hpp
- SurrogatesGPObjective.cpp

14.88 Graphics Class Reference

The Graphics class provides a single interface to 2D (motif) and 3D (PLPLOT) graphics; there is only one instance of this OutputManager::dakotaGraphics.

Public Member Functions

- Graphics ()

  constructor
- ~Graphics ()

  destructor
- void create_plots_2d (const Variables &vars, const Response &response)

creates the 2d graphics window and initializes the plots

- void add_datapoint (int graphics_cntr, const Variables &vars, const Response &response)

  adds data to each window in the 2d graphics based on the results of a model evaluation
- void add_datapoint (int i, double x, double y)

  adds data to a single window in the 2d graphics
- void new_dataset (int i)

  creates a separate line graphic for subsequent data points for a single window in the 2d graphics
- void close ()

  close graphics windows
- void set_x_labels2d (const char ∗x_label)

  set x label for each plot equal to x_label
- void set_y_labels2d (const char ∗y_label)

  set y label for each plot equal to y_label
- void set_x_label2d (int i, const char ∗x_label)

  set x label for ith plot equal to x_label
- void set_y_label2d (int i, const char ∗y_label)

  set y label for ith plot equal to y_label

Private Attributes

- Graphics2D ∗ graphics2D

  pointer to the 2D graphics object
- bool win2dOn

  flag to indicate if 2D graphics window is active

14.88.1 Detailed Description

The Graphics class provides a single interface to 2D (motif) and 3D (PLPLOT) graphics; there is only one instance of this OutputManager::dakotaGraphics.

14.88.2 Member Function Documentation

14.88.2.1 void create_plots_2d (const Variables & *vars*, const Response & *response*)

creates the 2d graphics window and initializes the plots

Sets up a single event loop for duration of the dakotaGraphics object, continuously adding data to a single window. There is no reset. To start over with a new data set, you need a new object (delete old and instantiate new).

References Variables::continuous_variable_labels(), Variables::cv(), Variables::discrete_int_variable_labels(), Variables::discrete_real_variable_labels(), Variables::div(), Variables::drv(), Response::function_labels(), Graphics::graphics2D, Response::num_functions(), Dakota::re_match(), and Graphics::win2dOn.

Referenced by Model::create_2d_plots().

14.88.2.2 void add_datapoint (int *graphics_cntr*, const Variables & *vars*, const Response & *response*)

adds data to each window in the 2d graphics based on the results of a model evaluation

Adds data to each 2d plot and each tabular data column (one for each active variable and for each response function). graphicsCntr is used for the x axis in the graphics and the first column in the tabular data.

References Response::active_set_request_vector(), Variables::continuous_variables(), Variables::discrete_int_variables(), Variables::discrete_real_variables(), Response::function_values(), Graphics::graphics2D, and Graphics::win2dOn.

Referenced by OutputManager::add_tabular_data(), NonDLocalReliability::mean_value(), and NonDLocal-Reliability::update_level_data().

14.88.2.3 void add_datapoint (int *i,* double *x,* double *y*)

adds data to a single window in the 2d graphics

Adds data to a single 2d plot. Allows complete flexibility in defining other kinds of x-y plotting in the 2D graphics.

References Graphics::graphics2D, and Graphics::win2dOn.

14.88.2.4 void new_dataset (int *i*)

creates a separate line graphic for subsequent data points for a single window in the 2d graphics

Used for displaying multiple data sets within the same plot.

References Graphics::graphics2D, and Graphics::win2dOn.

Referenced by NonDLocalReliability::update_level_data().

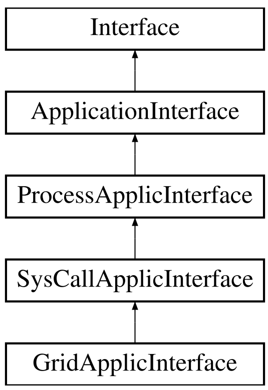
The documentation for this class was generated from the following files:

- DakotaGraphics.hpp
- DakotaGraphics.cpp

14.89 GridApplicInterface Class Reference

Derived application interface class which spawns simulation codes using grid services such as Condor or Globus.

Inheritance diagram for GridApplicInterface:



Public Member Functions

- GridApplicInterface (const ProblemDescDB &problem_db)

  constructor
- ∼GridApplicInterface ()

  destructor
- void derived_map (const Variables &vars, const ActiveSet &set, Response &response, int fn_eval_id)

  Called by map() and other functions to execute the simulation in synchronous mode. The portion of performing an evaluation that is specific to a derived class.
- void derived_map_asynch (const ParamResponsePair &pair)

Called by map() and other functions to execute the simulation in asynchronous mode. The portion of performing an asynchronous evaluation that is specific to a derived class.

- void wait_local_evaluation_sequence (PRPQueue &prp_queue)

  version of wait_local_evaluations() managing of set of individual asynchronous evaluations
- void test_local_evaluation_sequence (PRPQueue &prp_queue)

  Convenience function for common code between wait and nowait case.
- int synchronous_local_analysis (int analysis_id)

Protected Member Functions

- bool grid_file_test (const String &root_file)

  test file(s) for existence based on root_file name

Protected Attributes

- IntSet idSet

  Set of function evaluation id's for active asynchronous system call evaluations.
- IntShortMap failCountMap

  map linking function evaluation id's to number of response read failures
- start_grid_computing_t start_grid_computing

  handle to dynamically linked start_grid_computing function
- perform_analysis_t perform_analysis

  handle to dynamically linked perform_analysis grid function
- get_jobs_completed_t get_jobs_completed

  handle to dynamically linked get_jobs_completed grid function
- stop_grid_computing_t stop_grid_computing

  handle to dynamically linked stop_grid_computing function

14.89.1 Detailed Description

Derived application interface class which spawns simulation codes using grid services such as Condor or Globus.

This class is currently a modified copy of SysCallApplicInterface adapted for use with an external grid devices library which was dynamically linked using dlopen() services.

14.89.2 Member Function Documentation

14.89.2.1 int synchronous_local_analysis (int *analysis_id*) [inline], [virtual]

This code provides the derived function used by ApplicationInterface::serve_analyses_synch(). TODO - allow local analyses?????

Reimplemented from ApplicationInterface.

References SysCallApplicInterface::spawn_analysis_to_shell().

The documentation for this class was generated from the following files:

- GridApplicInterface.hpp
- GridApplicInterface.cpp

14.90 HDF5IOHelper Class Reference

Public Member Functions

- **HDF5IOHelper** (const std::string &file_name, bool overwrite=false)
- template< typename T >
  void store_scalar (const std::string &dset_name, const T &val)

  Store scalar data to a data set.
- void store_scalar (const std::string &dset_name, const String &val)

  Store string scalar data to a data set.
- template< typename T >
  void store_vector (const std::string &dset_name, const std::vector< T > &array) const

  Store vector (1D) information to a dataset.
- template< typename T >
  void store_vector (const std::string &dset_name, const Teuchos::SerialDenseVector< int, T > &vec)

  Store vector (1D) information to a dataset.
- void store_vector (const std::string &dset_name, const StringMultiArrayConstView &vec)

  Store vector (1D) information to a dataset.
- void store_vector (const std::string &dset_name, const SizetMultiArrayConstView &vec)

  Store vector (1D) information to a dataset.
- template< typename T >
  void store_matrix (const std::string &dset_name, const Teuchos::SerialDenseMatrix< int, T > &matrix, const bool &transpose=false) const

  Store matrix (2D) information to a dataset.
- template< typename T >
  void store_matrix (const std::string &dset_name, const std::vector< T > &buf, const int &num_cols, const bool &transpose=false) const

  Store matrix (2D) information to a dataset.
- void store_matrix (const std::string &dset_name, const std::vector< String > &buf, const int &num_cols, const bool &transpose=false) const

  Store matrix (2D) information to a dataset.
- template< typename T >
  void set_scalar (const String &dset_name, const T &data, const int &index)

  Set a scalar in a 1D dataset at index using its name.
- template< typename T >
  void set_scalar (const String &dset_name, H5::DataSet &ds, const T &data, const int &index)

  Set a scalar in a 1D dataset at index using the dataset object.
- void set_scalar (const String &dset_name, H5::DataSet &ds, const String &data, const int &index)

  Set a scalar in a 1D dataset at index using the dataset object.
- template< typename T >
  void set_vector (const String &dset_name, const T &data, const int &index, const bool &row=true)

  Set a row or column in a 2D dataset at index using its name.
- void set_vector (const String &dset_name, H5::DataSet &ds, const StringMultiArrayConstView &data, const int &index, const bool &row=true)

  Set a row or column of Strings in a 2D dataset at index using the dataset object.
- void set_vector (const String &dset_name, H5::DataSet &ds, const std::vector< String > &data, const int &index, const bool &row=true)

  Set a row or column of Strings in a 2D dataset at index using the dataset object.
- template< typename T >
  void set_vector (const String &dset_name, H5::DataSet &ds, const T &data, const int &index, const bool &row=true)

  Set a row or column in a 2D dataset at index using the dataset object.

- template<typename T >
  void set_matrix (const String &dset_name, const Teuchos::SerialDenseMatrix< int, T > &data, const int &index, const bool &transpose=false)

  Set a matrix in a 3D dataset at the index into the 0th dimension by name. Dims of matrix must match those of the trailing dimensions of the dataset.
- template<typename T >
  void set_matrix (const String &dset_name, H5::DataSet &ds, const Teuchos::SerialDenseMatrix< int, T > &data, const int &index, const bool &transpose=false)

  Set a matrix in a 3D dataset at the index into the 0th dimension using a dataset object. Dims of matrix must match those of the trailing dimensions of the dataset.
- template<typename T >
  void set_vector_matrix (const String &dset_name, const std::vector< Teuchos::SerialDenseMatrix< int, T > > &data, const int &index, const bool &transpose=false)

  Set a 3D slab in a 4D dataset at the index into the 0th dimension by name. The length of the vector must match the 1st dimension of the dataset, and the dimensions of the matrices must all match the 2nd and 3rd dimensions.
- template<typename T >
  void set_vector_matrix (const String &dset_name, H5::DataSet &ds, const std::vector< Teuchos::SerialDenseMatrix< int, T > > &data, const int &index, const bool &transpose=false)

  Set a 3D slab in a 4D dataset at the index into the 0th dimension using a dataset object. The length of the vector must match the 1st dimension of the dataset, and the dimensions of the matrices must all match the 2nd and 3rd dimensions.
- template<typename T >
  void set_vector_scalar_field (const String &dset_name, const T &data, const String &field_name)

  Set a scalar field on all elements of a 1D dataset of compound type using a ds name.
- template<typename T >
  void set_vector_scalar_field (const String &dset_name, H5::DataSet &ds, const std::vector< T > &data, const String &field_name)

  Set a scalar field on all elements of a 1D dataset of compound type using a ds object.
- template<typename T >
  void set_vector_vector_field (const String &dset_name, const T &data, const size_t length, const String &field_name)

  Set a vector field on all elements of a 1D dataset of compound type using a ds name.
- template<typename T >
  void set_vector_vector_field (const String &dset_name, H5::DataSet &ds, const std::vector< T > &data, const size_t length, const String &field_name)

  Set a vector field on all elements of a 1D dataset of compound type using a ds object.
- void set_vector_vector_field (const String &dset_name, H5::DataSet &ds, const std::vector< String > &data, const size_t length, const String &field_name)

  Set a vector field on all elements of a 1D dataset of compound type using a ds object.
- int append_empty (const String &dset_name)

  Append an empty "layer" to the 0th dimension and return its index.
- template<typename T >
  void append_scalar (const String &dset_name, const T &data)

  Append a scalar to a 1D dataset.
- void append_scalar (const String &dset_name, const String &data)

  Append a scalar to a 1D dataset.
- template<typename T >
  void append_vector (const String &dset_name, const T &data, const bool &row=true)

  Append a vector as a row or column to a 2D dataset.
- void append_vector (const String &dset_name, const std::vector< String > &data, const bool &row=true)

  Append a vector as a row or column to a 2D dataset.
- void append_vector (const String &dset_name, const StringMultiArrayConstView &data, const bool &row=true)

  Append a vector as a row or column to a 2D dataset.

- template<typename T >
void append_matrix (const String &dset_name, const Teuchos::SerialDenseMatrix< int, T > &data, const bool &transpose=false)

    Append a SerialDenseMatrix to a 3D dataset. The dataset will be expanded along the 0th dimension. By default, the shape of the matrix, (nrows, ncols), must match the size of the 1st and 2nd dimensions of the dataset. For transpose=true, the reverse must be true.

- template<typename T >
void append_vector_matrix (const String &dset_name, const std::vector< Teuchos::SerialDenseMatrix< int, T > > &data, const bool &transpose=false)

    Append a std::vector of SerialDenseMatrix's to a 4D dataset. The dataset will be expanded along the 0th dimension. By default, the size of the vector must equal the size of the 1st dimension of the dataset, andthe shape of the SDMs (nrows, ncols), must match the sizes of the 2nd and 2nd dimensions of the dataset. For transpose=true, the reverse must be true of the SDMs.

- template<typename T >
void read_scalar (const std::string &dset_name, T &val)

    Read scalar data from a dataset.

- void read_scalar (const std::string &dset_name, String &val)

    Read scalar data from a dataset.

- template<typename T >
void read_vector (const std::string &dset_name, T &array) const

    Read vector (1D) information from a dataset.

- void read_vector (const std::string &dset_name, StringArray &array) const

    Read a vector of Strings from a dataset.

- template<typename T >
void read_matrix (const std::string &dset_name, Teuchos::SerialDenseMatrix< int, T > &matrix, const bool &transpose=false) const

    Read matrix (2D) information from a dataset Currently this involves a wasteful copy to do the transpose and is intended only for purposes of testing.

- template<typename T >
void get_matrix (const std::string &dset_name, Teuchos::SerialDenseMatrix< int, T > &matrix, const int &index, const bool &transpose=false) const

    Get the matrix (2D) at the index into the 0th dimension of the 3D dataset at dsetname. Currently this involves a wasteful copy to do the transpose and is intended only for purposes of testing.

- template<typename T >
void get_vector_matrix (const std::string &dset_name, std::vector< Teuchos::SerialDenseMatrix< int, T > > &data, const int &index, const bool &transpose=false) const

    Read the 3D slice at the index into the 0th dimension of the 4D dataset at ds_name. Currently this involves a wasteful copy to do the transpose and is intended only for purposes of testing.

- void report_num_open ()

    Report the number of open descriptors of each type; just for debugging.

- void create_empty_dataset (const String &dset_name, const IntArray &dims, ResultsOutputType stored_type, int chunk_size=0, const void ∗fill_val=NULL)

    Create an empty dataset. Setting the first element of dims to 0 makes the dataset unlimited in that dimension. DSs unlimited in other dimensions currently are unsupported.

- void create_empty_dataset (const String &dset_name, const IntArray &dims, const std::vector< VariableParametersField > &fields)

    Create a dataset with compound type.

- void attach_scale (const String &dset_name, const String &scale_name, const String &label, const int &dim) const

    attach a dimension scale to a dataset

- template<typename T >
void add_attribute (const String &location, const String &label, const T &value)

    Add an attribute to a group or dataset.

- void add_attribute (const String &location, const String &label, const String &value)

    Add an attribute to a group or dataset.

- bool exists (const String location_name) const

    Does a group or dataset exist?
- bool is_scale (const H5::DataSet dset) const

    Is the dataset a dimenions scale?
- H5::Group create_groups (const std::string &name, bool includes_dset=true) const

    Create a group hierarchy (final token optionally a dataset name)
- H5::DataSet create_dataset (const H5::H5Location &loc, const std::string &name, const H5::DataType &type, const H5::DataSpace &space, const H5::DSetCreatPropList &create_plist=H5::DSetCreatPropList(), const H5::DSetAccPropList &access_plist=H5::DSetAccPropList()) const

    Create a dataset with a custom CreatPropList.
- H5::Group create_group (const H5::H5Location &loc, const std::string &name) const

    Create a group.
- void create_softlink (const String &link_location, const String &source_location)

    Create a soft link.
- void flush () const

    Flush cache to file.

Public Attributes

- H5::LinkCreatPropList linkCreatePL

    Gobal link creation property list.
- H5::DSetCreatPropList datasetCompactPL

    Gobal DataSet creation property list for compact datasets.
- H5::DSetCreatPropList datasetContiguousPL

    Gobal DataSet creation property list for contiguous datasets.

Protected Member Functions

- template<typename T >
  H5::Attribute create_attribute (const String &location, const String &label, const T &data)

    create an attribute at the location and return it
- template<typename T >
  void store_vector (const String &dset_name, const T ∗data, const int &len) const

    Store vector data using a pointer to the first element and length.
- void store_vector (const String &dset_name, const String ∗data, const int &len) const

    Store vector of Strings using a pointer to the first element and length.

Protected Attributes

- std::string fileName

    Name of the HDF5 file.
- H5::H5File h5File

    HDF5 file object.
- std::map< String, H5::DataSet > datasetCache

    Cache open datasets that have unlimited dimension This is an optimization to prevent eval-related datasets being repeatedly flushed and reopened, which is very costly.

14.90.1 Detailed Description

This helper class provides wrapper functions that perform low-level access operations in HDF5 databases.

Authors: J. Adam Stephens, Russell Hooper, Elliott Ridgway

14.90.2 Member Function Documentation

14.90.2.1 void set_scalar (const String & *dset_name,* H5::DataSet & *ds,* const String & *data,* const int & *index*)

Set a scalar in a 1D dataset at index using the dataset object.

Set a scalar in a 1D dataset at index using an object.

14.90.2.2 void set_vector_scalar_field (const String & *dset_name,* H5::DataSet & *ds,* const std::vector< T > & *data,* const String & *field_name*)

Set a scalar field on all elements of a 1D dataset of compound type using a ds object.

Set a field on all elements of a 1D dataset of compound type using a ds object.

References Dakota::h5_mem_dtype().

14.90.2.3 void set_vector_vector_field (const String & *dset_name,* H5::DataSet & *ds,* const std::vector< T > & *data,* const size_t *length,* const String & *field_name*)

Set a vector field on all elements of a 1D dataset of compound type using a ds object.

Set a field on all elements of a 1D dataset of compound type using a ds object.

References Dakota::h5_mem_dtype().

14.90.2.4 void set_vector_vector_field (const String & *dset_name,* H5::DataSet & *ds,* const std::vector< String > & *data,* const size_t *length,* const String & *field_name*)

Set a vector field on all elements of a 1D dataset of compound type using a ds object.

Set a field on all elements of a 1D dataset of compound type using a ds object.

References Dakota::pointers_to_strings().

14.90.2.5 void read_vector (const std::string & *dset_name,* StringArray & *array*) const

Read a vector of Strings from a dataset.

Read vector (1D) String information from a dataset.

References Dakota::abort_handler(), and Dakota::h5_mem_dtype().

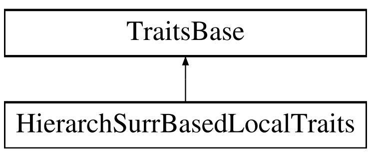
The documentation for this class was generated from the following files:

- HDF5_IO.hpp
- HDF5_IO.cpp

14.91 HierarchSurrBasedLocalTraits Class Reference

Class for multilevel-multifidelity optimization algorithm.

Inheritance diagram for HierarchSurrBasedLocalTraits:



Public Member Functions

- HierarchSurrBasedLocalTraits ()

    default constructor
- virtual ∼HierarchSurrBasedLocalTraits ()

    destructor
- virtual bool is_derived ()

    A temporary query used in the refactor.
- bool supports_continuous_variables ()

    Return the flag indicating whether method supports continuous variables.
- bool supports_linear_equality ()

    Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()

    Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()

    Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

    Return the flag indicating whether method supports nonlinear inequalities.

14.91.1 Detailed Description

Class for multilevel-multifidelity optimization algorithm.

This minimizer uses SurrogateModel(s) to perform minimization leveraging multiple model forms and discretization levels. A version of TraitsBase specialized for multilevel-multifidelity minimizer

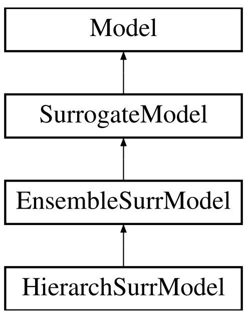
The documentation for this class was generated from the following file:

- HierarchSurrBasedLocalMinimizer.hpp

14.92 HierarchSurrModel Class Reference

Derived model class within the surrogate model branch for managing hierarchical surrogates (models of varying fidelity).

Inheritance diagram for HierarchSurrModel:



Public Member Functions

- HierarchSurrModel (ProblemDescDB &problem_db)

    constructor
- ∼HierarchSurrModel ()

destructor
- const unsigned short correction_mode () const

  return correctionMode
- void correction_mode (unsigned short corr_mode)

  set correctionMode

Protected Member Functions

- bool initialize_mapping (ParLevLIter pl_iter)
- bool finalize_mapping ()
- void derived_evaluate (const ActiveSet &set)
- void derived_evaluate_nowait (const ActiveSet &set)
- void **derived_synchronize_sequential** (IntResponseMapArray &model_resp_maps_rekey, bool block)
- void **derived_synchronize_combine** (IntResponseMapArray &model_resp_maps, IntResponseMap &combined_resp_map)
- void **derived_synchronize_combine_nowait** (IntResponseMapArray &model_resp_maps, IntResponseMap &combined_resp_map)
- size_t num_approximation_models () const

  return the number of models that approximate the truth model
- void assign_default_keys ()

  initialize truth and surrogate model keys to default values
- void resize_maps ()

  size id_maps and cached_resp_maps arrays according to responseMode
- void resize_response (bool use_virtual_counts=true)

  resize currentResponse based on responseMode
- size_t insert_response_start (size_t position)

  compute start index for inserting response data into aggregated response
- void insert_metadata (const RealArray &md, size_t position, Response &agg_response)

  insert a single response into an aggregated response in the specified position
- void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

  set primaryA{C,DI,DS,DR}VarMapIndices, secondaryA{C,DI,DS,DR}VarMapTargets (coming from a higher-level NestedModel context to inform derivative est.)
- DiscrepancyCorrection & discrepancy_correction ()

  return the DiscrepancyCorrection object used by SurrogateModels
- short correction_type ()

  return the correction type from the DiscrepancyCorrection object used by SurrogateModels
- void correction_type (short corr_type)

  set the correction type from the DiscrepancyCorrection object used by SurrogateModels
- short correction_order ()

  return the correction order from the DiscrepancyCorrection object used by SurrogateModels
- void create_tabular_datastream ()

  create a tabular output stream for automatic logging of vars/response data
- void derived_auto_graphics (const Variables &vars, const Response &resp)

  Update tabular/graphics data with latest variables/response data.
- Model & surrogate_model (size_t i=_NPOS)

  return the active low fidelity model
- const Model & surrogate_model (size_t i=_NPOS) const

  return the active low fidelity model
- Model & truth_model ()

  return the active high fidelity model

- const Model & truth_model () const

  return the active high fidelity model
- void active_model_key (const Pecos::ActiveKey &key)

  define the active model key and associated {truth,surr}ModelKey pairing
- void clear_model_keys ()

  remove keys for any approximations underlying orderedModels
- void derived_subordinate_models (ModelList &ml, bool recurse_flag)

  return orderedModels and, optionally, their sub-model recursions
- void resize_from_subordinate_model (size_t depth=SZ_MAX)

  resize currentResponse if needed when one of the subordinate models has been resized
- void update_from_subordinate_model (size_t depth=SZ_MAX)

  update currentVariables using non-active data from the passed model (one of the ordered models)
- void primary_response_fn_weights (const RealVector &wts, bool recurse_flag=true)

  set the relative weightings for multiple objective functions or least squares terms and optionally recurses into LF/HF models
- void surrogate_response_mode (short mode)

  set responseMode and pass any bypass request on to the high fidelity model for any lower-level surrogate recursions
- void build_approximation ()

  use the high fidelity model to compute the truth values needed for correction of the low fidelity model results
- void component_parallel_mode (short mode)

  update component parallel mode for supporting parallelism in the low ad high fidelity models
- IntIntPair estimate_partition_bounds (int max_eval_concurrency)

  estimate the minimum and maximum partition sizes that can be utilized by this Model
- void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set up parallel operations for the array of ordered model fidelities
- void derived_init_serial ()

  set up serial operations for the array of ordered model fidelities
- void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set active parallel configuration within the current low and high fidelity models identified by {low,high}FidelityKey
- void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  deallocate communicator partitions for the HierarchSurrModel (request forwarded to the the array of ordered model fidelities)
- void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)

  Service the low and high fidelity model job requests received from the master; completes when termination message received from stop_servers().
- void inactive_view (short view, bool recurse_flag=true)

  update the Model's inactive view based on higher level (nested) context and optionally recurse into
- bool evaluation_cache (bool recurse_flag=true) const

  if recurse_flag, return true if orderedModels evaluation cache usage
- bool restart_file (bool recurse_flag=true) const

  if recurse_flag, return true if orderedModels restart file usage
- void fine_grained_evaluation_counters ()

  request fine-grained evaluation reporting within the low and high fidelity models
- void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const

  print the evaluation summary for the HierarchSurrModel (request forwarded to the low and high fidelity models)
- void warm_start_flag (const bool flag)

  set the warm start flag, including the orderedModels

Private Member Functions

- void assign_truth_key ()

  synchronize the HF model's solution level control with truthModelKey
- void assign_surrogate_key ()

  synchronize the LF model's solution level control with surrModelKey
- void extract_model_keys (const Pecos::ActiveKey &active_key, Pecos::ActiveKey &truth_key, Pecos::ActiveKey &surr_key)

  define truth and surrogate keys from incoming active key. In case of singleton, use responseMode to disambiguate.
- void extract_model_keys (const Pecos::ActiveKey &active_key, Pecos::ActiveKey &truth_key, Pecos::ActiveKey &surr_key, short parallel_mode)

  define truth and surrogate keys from incoming active key. In case of singleton, use component parallel mode to disambiguate.
- bool matching_truth_surrogate_interface_ids ()

  check for matching interface ids among active truth/surrogate models (varies based on active keys)
- bool matching_all_interface_ids ()

  check for matching interface ids across full set of models (invariant)
- void check_model_interface_instance ()

  update sameInterfaceInstance based on interface ids for models identified by current {low,high}FidelityKey
- void compute_apply_delta (IntResponseMap &lf_resp_map)

  helper function used in the AUTO_CORRECTED_SURROGATE responseMode for computing a correction and applying it to lf_resp_map
- void single_apply (const Variables &vars, Response &resp, const Pecos::ActiveKey &paired_key)

  helper function for applying a single response correction corresponding to deltaCorr[paired_key]
- void recursive_apply (const Variables &vars, Response &resp)

  helper function for applying a correction across a sequence of model forms or discretization levels
- void stop_model (size_t ordered_model_index)

  stop the servers for the orderedModels instance identified by the passed index

Private Attributes

- std::map< Pecos::ActiveKey, DiscrepancyCorrection > deltaCorr

  manages construction and application of correction functions that are applied to a surrogate model (DataFitSurr or HierarchSurr) in order to reproduce high fidelity data.
- short corrOrder

  order of correction: 0, 1, or 2
- unsigned short **correctionMode**
- ModelArray orderedModels

  Ordered sequence (low to high) of model fidelities. Models are of arbitrary type and supports recursions.
- Pecos::ActiveKey surrModelKey

  key defining model form / resolution level for the active LF approximation
- Pecos::ActiveKey componentParallelKey

  store {LF,HF} model key that is active in component_parallel_mode()
- IntVariablesMap rawVarsMap

  map of raw continuous variables used by apply_correction(). Model::varsList cannot be used for this purpose since it does not contain lower level variables sets from finite differencing.
- std::map< Pecos::ActiveKey, Response > truthResponseRef

  map of reference truth (high fidelity) responses computed in build_approximation() and used for calculating corrections

Additional Inherited Members

14.92.1 Detailed Description

Derived model class within the surrogate model branch for managing hierarchical surrogates (models of varying fidelity).

The HierarchSurrModel class manages hierarchical models of varying fidelity. The class contains an ordered array of model forms (fidelity ordered from low to high), where each model form may also contain a set of solution levels (space/time discretization, convergence tolerances, etc.). At run time, one of these combinations is activated as the low fidelity model and used to perform approximate function evaluations, while another of these combinations is activated as the high fidelity model and used to provide truth evaluations for computing corrections to the low fidelity results.

14.92.2 Member Function Documentation

14.92.2.1 bool initialize_mapping (ParLevLIter *pl_iter*) [protected], [virtual]

Inactive variables must be propagated when a HierarchSurrModel is employed by a sub-iterator (e.g., OUU with MLMC or MLPCE). In current use cases, this can occur once per sub-iterator execution within Model::initialize_-mapping().

Reimplemented from Model.

References EnsembleSurrModel::init_model(), Model::initialize_mapping(), and HierarchSurrModel::ordered-Models.

14.92.2.2 bool finalize_mapping ( ) [protected], [virtual]

Inactive variables must be propagated when a HierarchSurrModel is employed by a sub-iterator (e.g., OUU with MLMC or MLPCE). In current use cases, this can occur once per sub-iterator execution within Model::initialize_-mapping().

Reimplemented from Model.

References Model::finalize_mapping(), and HierarchSurrModel::orderedModels.

14.92.2.3 void derived_evaluate (const ActiveSet & *set*) [protected], [virtual]

Compute the response synchronously using LF model, HF model, or both (mixed case). For the LF model portion, compute the high fidelity response if needed with build_approximation(), and, if correction is active, correct the low fidelity results.

Reimplemented from Model.

References Response::active_set(), SurrogateModel::activeKey, SurrogateModel::aggregate_response(), SurrogateModel::approxBuilds, HierarchSurrModel::assign_surrogate_key(), HierarchSurrModel::assign_truth_-key(), SurrogateModel::asv_split(), HierarchSurrModel::build_approximation(), HierarchSurrModel::component_-parallel_mode(), Response::copy(), Model::current_response(), Model::currentResponse, Model::currentVariables, HierarchSurrModel::deltaCorr, ActiveSet::derivative_vector(), Dakota::dummy_model, Model::eval_tag_prefix(), Model::evalTagPrefix, Model::evaluate(), SurrogateModel::force_rebuild(), Model::hierarchicalTagging, Model-::outputLevel, HierarchSurrModel::recursive_apply(), ActiveSet::request_vector(), SurrogateModel::response_-combine(), SurrogateModel::responseMode, EnsembleSurrModel::sameModelInstance, SurrogateModel::surr-ModelEvalCntr, HierarchSurrModel::surrogate_model(), HierarchSurrModel::truth_model(), Response::update(), and SurrogateModel::update_model().

14.92.2.4 void derived_evaluate_nowait (const ActiveSet & *set*) [protected], [virtual]

Compute the response asynchronously using LF model, HF model, or both (mixed case). For the LF model portion, compute the high fidelity response with build_approximation() (for correcting the low fidelity results in derived_synchronize() and derived_synchronize_nowait()) if not performed previously.

Reimplemented from Model.

References SurrogateModel::approxBuilds, HierarchSurrModel::assign_surrogate_key(), HierarchSurrModel::assign_truth_key(), SurrogateModel::asv_split(), Model::asynch_flag(), HierarchSurrModel::build_approximation(), EnsembleSurrModel::cachedRespMaps, HierarchSurrModel::component_parallel_mode(), Response::copy(), Variables::copy(), Model::current_response(), Model::currentVariables, ActiveSet::derivative_vector(), Dakota::dummy_model, Model::eval_tag_prefix(), Model::evalTagPrefix, Model::evaluate(), Model::evaluate_nowait(), Model::evaluation_id(), SurrogateModel::force_rebuild(), Model::hierarchicalTagging, EnsembleSurrModel::modelIdMaps, HierarchSurrModel::rawVarsMap, HierarchSurrModel::recursive_apply(), ActiveSet::request_vector(), SurrogateModel::responseMode, EnsembleSurrModel::sameModelInstance, SurrogateModel::surrModelEvalCntr, HierarchSurrModel::surrogate_model(), HierarchSurrModel::truth_model(), and SurrogateModel::update_model().

The documentation for this class was generated from the following files:

- HierarchSurrModel.hpp
- HierarchSurrModel.cpp

14.93 IntegerScale Struct Reference

Data structure for storing int-valued dimension scale.

Public Member Functions

- IntegerScale (const std::string &label, const IntVector &in_items, ScaleScope scope=ScaleScope::UNSHARED)

    Constructor that takes an IntVector.
- IntegerScale (const std::string &label, const IntArray &in_items, ScaleScope scope=ScaleScope::UNSHARED)

    Constructor that takes an IntArray.
- IntegerScale (const std::string &label, const int ∗in_items, const int len, ScaleScope scope=ScaleScope::UNSHARED)

    Constructor that takes a pointer to int and length.
- IntegerScale (const std::string &in_label, std::initializer_list< int > in_items, ScaleScope in_scope=ScaleScope::UNSHARED)

    Constructor that takes an initializer_list.

Public Attributes

- std::string **label**
- ScaleScope **scope**
- IntVector **items**
- int numCols

    Number of columns; equals length of scale when 1D.
- bool isMatrix

    2d or 1d?

14.93.1 Detailed Description

Data structure for storing int-valued dimension scale.

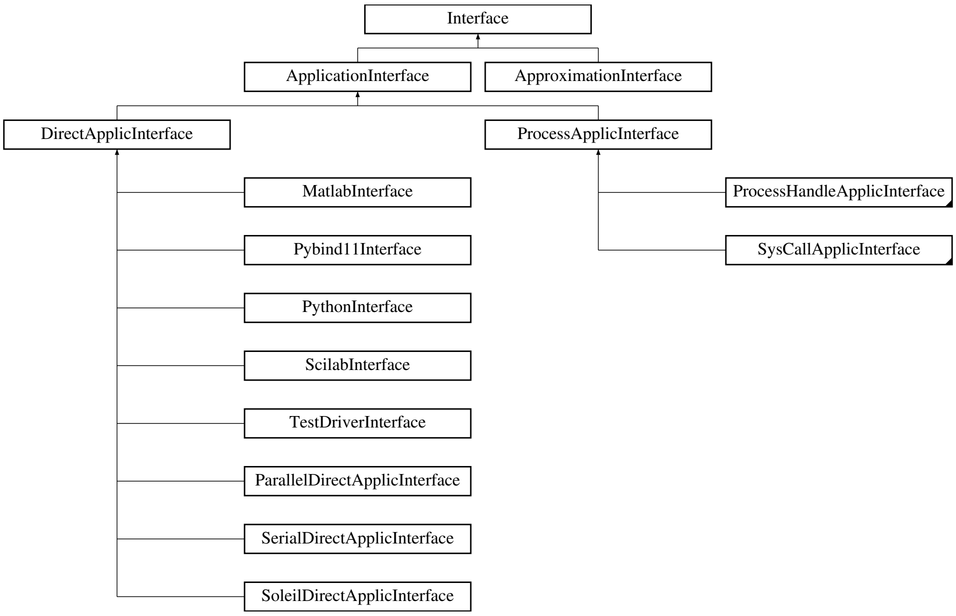
The documentation for this struct was generated from the following file:

- dakota_results_types.hpp

14.94 Interface Class Reference

Base class for the interface class hierarchy.

Inheritance diagram for Interface:



Public Member Functions

- Interface ()

    default constructor
- Interface (ProblemDescDB &problem_db)

    standard constructor for envelope
- Interface (const Interface &interface_in)

    copy constructor
- virtual ~Interface ()

    destructor
- Interface operator= (const Interface &interface_in)

    assignment operator
- virtual void map (const Variables &vars, const ActiveSet &set, Response &response, bool asynch_flag=false)

    the function evaluator: provides a "mapping" from the variables to the responses.
- virtual const IntResponseMap & synchronize ()

    recovers data from a series of asynchronous evaluations (blocking)
- virtual const IntResponseMap & synchronize_nowait ()

    recovers data from a series of asynchronous evaluations (nonblocking)
- virtual void serve_evaluations ()

evaluation server function for multiprocessor executions

- virtual void stop_evaluation_servers ()

  send messages from iterator rank 0 to terminate evaluation servers
- virtual void init_communicators (const IntArray &message_lengths, int max_eval_concurrency)

  allocate communicator partitions for concurrent evaluations within an iterator and concurrent multiprocessor analyses within an evaluation.
- virtual void set_communicators (const IntArray &message_lengths, int max_eval_concurrency)

  set the local parallel partition data for an interface (the partitions are already allocated in ParallelLibrary).
- virtual void init_serial ()

  reset certain defaults for serial interface objects.
- virtual int asynch_local_evaluation_concurrency () const

  return the user-specified concurrency for asynch local evaluations
- virtual short interface_synchronization () const

  return the user-specified interface synchronization
- virtual int minimum_points (bool constraint_flag) const

  returns the minimum number of points required to build a particular ApproximationInterface (used by DataFitSurrModels).
- virtual int recommended_points (bool constraint_flag) const

  returns the recommended number of points required to build a particular ApproximationInterface (used by DataFitSurrModels).
- virtual void active_model_key (const Pecos::ActiveKey &key)

  activate an approximation state based on its key
- virtual void clear_model_keys ()

  reset initial state by removing all model keys for an approximation
- virtual void approximation_function_indices (const SizetSet &approx_fn_indices)

  set the (currently active) approximation function index set
- virtual void update_approximation (const Variables &vars, const IntResponsePair &response_pr)

  updates the anchor point for an approximation
- virtual void update_approximation (const RealMatrix &samples, const IntResponseMap &resp_map)

  updates the current data points for an approximation
- virtual void update_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map)

  updates the current data points for an approximation
- virtual void append_approximation (const Variables &vars, const IntResponsePair &response_pr)

  appends a single point to an existing approximation
- virtual void append_approximation (const RealMatrix &samples, const IntResponseMap &resp_map)

  appends multiple points to an existing approximation
- virtual void append_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map)

  appends multiple points to an existing approximation
- virtual void append_approximation (const IntVariablesMap &vars_map, const IntResponseMap &resp_map)

  appends multiple points to an existing approximation
- virtual void replace_approximation (const IntResponsePair &response_pr)

  replace the response for a single point within an existing approximation
- virtual void replace_approximation (const IntResponseMap &resp_map)

  replace responses for multiple points within an existing approximation
- virtual void track_evaluation_ids (bool track)

  assigns trackEvalIds to activate tracking of evaluation ids within surrogate data, enabling id-based lookups for data replacement
- virtual void build_approximation (const RealVector &c_l_bnds, const RealVector &c_u_bnds, const IntVector &di_l_bnds, const IntVector &di_u_bnds, const RealVector &dr_l_bnds, const RealVector &dr_u_bnds)

  builds the approximation
- virtual void export_approximation ()

  export the approximation to disk

- virtual void rebuild_approximation (const BitArray &rebuild_fns)
  rebuilds the approximation after a data update
- virtual void pop_approximation (bool save_data)
  removes data from last append from the approximation
- virtual void push_approximation ()
  retrieves approximation data from a previous state (negates pop)
- virtual bool push_available ()
  queries the approximation for the ability to retrieve a previous increment
- virtual void finalize_approximation ()
  finalizes the approximation by applying all trial increments
- virtual void combine_approximation ()
  combine the current approximation with previously stored data sets
- virtual void combined_to_active (bool clear_combined=true)
  promote the combined approximation to the currently active one
- virtual void clear_inactive ()
  clear inactive approximation data
- virtual bool advancement_available ()
  query for available advancements in approximation resolution controls
- virtual bool formulation_updated () const
  query for change in approximation formulation
- virtual void formulation_updated (bool update)
  assign an updated status for approximation formulation to force rebuild
- virtual Real2DArray cv_diagnostics (const StringArray &metric_types, unsigned num_folds)
  approximation cross-validation quality metrics per response function
- virtual RealArray challenge_diagnostics (const String &metric_type, const RealMatrix &challenge_pts)
  approximation challenge data metrics per response function
- virtual void clear_current_active_data ()
  clears current data from an approximation interface
- virtual void clear_active_data ()
  clears all data from an approximation interface
- virtual SharedApproxData & shared_approximation ()
  retrieve the SharedApproxData within an ApproximationInterface
- virtual std::vector
  < Approximation > & approximations ()
  retrieve the Approximations within an ApproximationInterface
- virtual const
  Pecos::SurrogateData & approximation_data (size_t fn_index)
  retrieve the approximation data from a particular Approximation within an ApproximationInterface
- virtual const RealVectorArray & approximation_coefficients (bool normalized=false)
  retrieve the approximation coefficients from each Approximation within an ApproximationInterface
- virtual void approximation_coefficients (const RealVectorArray &approx_coeffs, bool normalized=false)
  set the approximation coefficients within each Approximation within an ApproximationInterface
- virtual const RealVector & approximation_variances (const Variables &vars)
  retrieve the approximation variances from each Approximation within an ApproximationInterface
- virtual const StringArray & analysis_drivers () const
  retrieve the analysis drivers specification for application interfaces
- virtual const String2DArray & analysis_components () const
  retrieve the analysis components, if available
- virtual bool evaluation_cache () const
  return flag indicating usage of the global evaluation cache
- virtual bool restart_file () const

return flag indicating usage of the restart file
- virtual void file_cleanup () const

  clean up any interface parameter/response files when aborting
- IntResponseMap & response_map ()

  return rawResponseMap
- void cache_unmatched_response (int raw_id)

  migrate an unmatched response record from rawResponseMap to cachedResponseMap
- void cache_unmatched_responses ()

  migrate all remaining response records from rawResponseMap to cachedResponseMap
- void assign_rep (std::shared_ptr< Interface > interface_rep)

  assign letter or replace existing letter with a new one
- void assign_rep (Interface ∗interface_rep, bool ref_count_incr=false)

  assign letter or replace existing letter with a new one DEPRECATED, but left for library mode clients to migrate: transfers memory ownership to the contained shared_ptr; ref_count_incr is ignored
- unsigned short interface_type () const

  returns the interface type
- const String & interface_id () const

  returns the interface identifier
- int evaluation_id () const

  returns the value of the (total) evaluation id counter for the interface
- void fine_grained_evaluation_counters (size_t num_fns)

  set fineGrainEvalCounters to true and initialize counters if needed
- void init_evaluation_counters (size_t num_fns)

  initialize fine grained evaluation counters, sizing if needed
- void set_evaluation_reference ()

  set evaluation count reference points for the interface
- void print_evaluation_summary (std::ostream &s, bool minimal_header, bool relative_count) const

  print an evaluation summary for the interface
- bool multi_proc_eval () const

  returns a flag signaling the use of multiprocessor evaluation partitions
- bool iterator_eval_dedicated_master () const

  returns a flag signaling the use of a dedicated master processor at the iterator-evaluation scheduling level
- bool is_null () const

  function to check interfaceRep (does this envelope contain a letter?)
- std::shared_ptr< Interface > interface_rep ()

  function to return the letter
- void eval_tag_prefix (const String &eval_id_str, bool append_iface_id=true)

  set the evaluation tag prefix (does not recurse)

Protected Member Functions

- Interface (BaseConstructor, const ProblemDescDB &problem_db)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- Interface (NoDBBaseConstructor, size_t num_fns, short output_level)

  constructor initializes the base class part of letter classes (NoDBBaseConstructor used for on the fly instantiations without a DB)
- void init_algebraic_mappings (const Variables &vars, const Response &response)

  Define algebraicACVIndices, algebraicACVIds, and algebraicFnIndices.
- void asv_mapping (const ActiveSet &total_set, ActiveSet &algebraic_set, ActiveSet &core_set)

define the evaluation requirements for algebraic_mappings() (algebraic_set) and the core Application/Approximation mapping (core_set) from the total Interface evaluation requirements (total_set)

- void asv_mapping (const ActiveSet &algebraic_set, ActiveSet &total_set)

  map an algebraic ASV back to original total ordering for asynch recovery
- void algebraic_mappings (const Variables &vars, const ActiveSet &algebraic_set, Response &algebraic_response)

  evaluate the algebraic_response using the AMPL solver library and the data extracted from the algebraic_mappings file
- void response_mapping (const Response &algebraic_response, const Response &core_response, Response &total_response)

  combine the response from algebraic_mappings() with the response from derived_map() to create the total response
- virtual String final_eval_id_tag (int fn_eval_id)

  form and return the final evaluation ID tag, appending iface ID if needed

Protected Attributes

- unsigned short interfaceType

  the interface type: enum for system, fork, direct, grid, or approximation
- String interfaceId

  the interface specification identifier string from the DAKOTA input file
- bool algebraicMappings

  flag for the presence of algebraic_mappings that define the subset of an Interface's parameter to response mapping that is explicit and algebraic.
- bool coreMappings

  flag for the presence of non-algebraic mappings that define the core of an Interface's parameter to response mapping (using analysis_drivers for ApplicationInterface or functionSurfaces for ApproximationInterface).
- short outputLevel

  output verbosity level: {SILENT,QUIET,NORMAL,VERBOSE,DEBUG}_OUTPUT
- int currEvalId

  identifier for the current evaluation, which may differ from the evaluation counters in the case of evaluation scheduling; used on iterator master as well as server processors. Currently, this is set prior to all invocations of derived_map() for all processors.
- bool fineGrainEvalCounters

  controls use of fn val/grad/hess counters for detailed evaluation report
- int evalIdCntr

  total interface evaluation counter
- int newEvalIdCntr

  new (non-duplicate) interface evaluation counter
- int evalIdRefPt

  iteration reference point for evalIdCntr
- int newEvalIdRefPt

  iteration reference point for newEvalIdCntr
- IntArray fnValCounter

  number of value evaluations by resp fn
- IntArray fnGradCounter

  number of gradient evaluations by resp fn
- IntArray fnHessCounter

  number of Hessian evaluations by resp fn
- IntArray newFnValCounter

  number of new value evaluations by resp fn
- IntArray newFnGradCounter

  number of new gradient evaluations by resp fn

- IntArray newFnHessCounter

  number of new Hessian evaluations by resp fn
- IntArray fnValRefPt

  iteration reference point for fnValCounter
- IntArray fnGradRefPt

  iteration reference point for fnGradCounter
- IntArray fnHessRefPt

  iteration reference point for fnHessCounter
- IntArray newFnValRefPt

  iteration reference point for newFnValCounter
- IntArray newFnGradRefPt

  iteration reference point for newFnGradCounter
- IntArray newFnHessRefPt

  iteration reference point for newFnHessCounter
- IntResponseMap rawResponseMap

  Set of responses returned by either a blocking or nonblocking schedule.
- IntResponseMap cachedResponseMap

  Set of available asynchronous responses completed within a blocking or nonblocking scheduler that cannot be processed in a higher level context and need to be stored for later.
- StringArray fnLabels

  response function descriptors (used in print_evaluation_summary() and derived direct interface classes); initialized in map() functions due to potential updates after construction
- bool multiProcEvalFlag

  flag for multiprocessor evaluation partitions (evalComm)
- bool ieDedMasterFlag

  flag for dedicated master partitioning at the iterator level
- String evalTagPrefix

  set of period-delimited evaluation ID tags to use in evaluation tagging
- bool appendIfaceId

  whether to append the interface ID to the prefix during map (default true)
- String2DArray analysisComponents

  Analysis components for interface types that support them.

Private Member Functions

- std::shared_ptr< Interface > get_interface (ProblemDescDB &problem_db)

  Used by the envelope to instantiate the correct letter class.
- int algebraic_function_type (String)

  Used by algebraic mappings to determine the correct AMPL function evaluation call to make.

Static Private Member Functions

- static String user_auto_id ()

  return the next available interface ID for no-ID user methods
- static String no_spec_id ()

  return the next available interface ID for on-the-fly methods

Private Attributes

- StringArray algebraicVarTags
  set of variable tags from AMPL stub.col
- SizetArray algebraicACVIndices
  set of indices mapping AMPL algebraic variables to DAKOTA all continuous variables
- SizetArray algebraicACVIds
  set of ids mapping AMPL algebraic variables to DAKOTA all continuous variables
- StringArray algebraicFnTags
  set of function tags from AMPL stub.row
- IntArray algebraicFnTypes
  function type: $>$ 0 = objective, $<$ 0 = constraint $|$value$|$-1 is the objective (constraint) index when making AMPL objval (conival) calls
- SizetArray algebraicFnIndices
  set of indices mapping AMPL algebraic objective functions to DAKOTA response functions
- RealArray algebraicConstraintWeights
  set of weights for computing Hessian matrices for algebraic constraints;
- int numAlgebraicResponses
  number of algebraic responses (objectives+constraints)
- std::shared_ptr$<$ Interface $>$ interfaceRep
  pointer to the letter (initialized only for the envelope)
- ASL $*$ asl
  pointer to an AMPL solver library (ASL) object

Static Private Attributes

- static size_t noSpecIdNum = 0
  the last used interface ID number for on-the-fly instantiations (increment before each use)

14.94.1 Detailed Description

Base class for the interface class hierarchy.

The Interface class hierarchy provides the part of a Model that is responsible for mapping a set of Variables into a set of Responses. The mapping is performed using either a simulation-based application interface or a surrogate-based approximation interface. For memory efficiency and enhanced polymorphism, the interface hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Interface) serves as the envelope and one of the derived classes (selected in Interface::get_interface()) serves as the letter.

14.94.2 Constructor & Destructor Documentation

14.94.2.1 Interface ( )

default constructor

used in Model envelope class instantiations

14.94.2.2 Interface (ProblemDescDB & *problem_db*)

standard constructor for envelope

Used in Model instantiation to build the envelope. This constructor only needs to extract enough data to properly execute get_interface, since Interface::Interface(BaseConstructor, problem_db) builds the actual base class data inherited by the derived interfaces.

References Dakota::abort_handler(), and Interface::interfaceRep.

14.94.2.3 Interface (const Interface & *interface_in*)

copy constructor

Copy constructor manages sharing of interfaceRep

14.94.2.4 Interface (BaseConstructor , const ProblemDescDB & *problem_db*) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all inherited interfaces. get_interface() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid the recursion of the base class constructor calling get_interface() again). Since this is the letter and the letter IS the representation, interfaceRep is set to NULL.

References Dakota::abort_handler(), Interface::algebraic_function_type(), Interface::algebraicConstraintWeights, Interface::algebraicFnTags, Interface::algebraicFnTypes, Interface::algebraicMappings, Interface::algebraicVarTags, Interface::asl, ProblemDescDB::get_string(), Interface::interfaceId, Interface::outputLevel, Dakota::strends(), and Interface::user_auto_id().

14.94.3 Member Function Documentation

14.94.3.1 void assign_rep (std::shared_ptr< Interface > *interface_rep*)

assign letter or replace existing letter with a new one

The assign_rep() function is used for publishing derived class letters to existing envelopes, as opposed to sharing representations among multiple envelopes (in particular, assign_rep is passed a letter object and operator= is passed an envelope object).

Use case assumes the incoming letter is instantiated on the fly and has no envelope. This case is modeled after get_interface(): a letter is dynamically allocated and passed into assign_rep (its memory management is passed over to the envelope).

If the letter happens to be managed by another envelope, it will persist as long as the last envelope referencing it.

References Interface::interface_rep(), and Interface::interfaceRep.

Referenced by DataFitSurrModel::DataFitSurrModel(), parallel_interface_plugin(), LibraryEnvironment::plugin_interface(), and run_dakota().

14.94.3.2 void assign_rep (Interface ∗ *interface_rep*, bool *ref_count_incr* = false)

assign letter or replace existing letter with a new one DEPRECATED, but left for library mode clients to migrate: transfers memory ownership to the contained shared_ptr; ref_count_incr is ignored

DEPRECATED but temporarily left for library mode clients needing to MIGRATE TO shared_ptr API

Similar to the assignment operator, the assign_rep() function decrements referenceCount for the old interfaceRep and assigns the new interfaceRep. It is different in that it is used for publishing derived class letters to existing envelopes, as opposed to sharing representations among multiple envelopes (in particular, assign_rep is passed a letter object and operator= is passed an envelope object). Letter assignment historically supported two models as governed by ref_count_incr:

- ref_count_incr = true (removed): the incoming letter belongs to another envelope. In this case, increment the reference count in the normal manner so that deallocation of the letter is handled properly.

- ref_count_incr = false (always): the incoming letter is instantiated on the fly and has no envelope. This case is modeled after get_interface(): a letter is dynamically allocated using new and passed into assign_rep, the letter's reference count is not incremented, and the letter is not remotely deleted (its memory management is passed over to the envelope).

References Interface::interfaceRep.

14.94.3.3 void eval_tag_prefix (const String & *eval_id_str,* bool *append_iface_id* = true)

set the evaluation tag prefix (does not recurse)

default implementation just sets the list of eval ID tags; derived classes containing additional models or interfaces should override (currently no use cases)

References Interface::appendIfaceId, Interface::evalTagPrefix, and Interface::interfaceRep.

Referenced by NestedModel::derived_evaluate(), and SimulationModel::eval_tag_prefix().

14.94.3.4 void response_mapping (const Response & *algebraic_response,* const Response & *core_response,* Response & *total_response*) [protected]

combine the response from algebraic_mappings() with the response from derived_map() to create the total response

This function will get invoked even when only algebraic mappings are active (no core mappings from derived_-map), since the AMPL algebraic_response may be ordered differently from the total_response. In this case, the core_response object is unused.

References Dakota::abort_handler(), Response::active_set_derivative_vector(), Response::active_set_request_-vector(), Interface::algebraicACVIds, Interface::algebraicFnIndices, Interface::coreMappings, Dakota::find_index(), Response::function_gradient(), Response::function_gradient_view(), Response::function_gradients(), Response-::function_hessian(), Response::function_hessian_view(), Response::function_hessians(), Response::function-_value(), Response::function_values(), Response::function_values_view(), Interface::outputLevel, Response-::reset(), and Response::reset_inactive().

Referenced by ApproximationInterface::map(), ApplicationInterface::map(), ApplicationInterface::synchronize(), and ApplicationInterface::synchronize_nowait().

14.94.3.5 std::shared_ptr< Interface > get_interface (ProblemDescDB & *problem_db*) [private]

Used by the envelope to instantiate the correct letter class.

used only by the envelope constructor to initialize interfaceRep to the appropriate derived type.

References ProblemDescDB::get_string(), ProblemDescDB::get_ushort(), and Interface::interface_type().

14.94.3.6 String user_auto_id ( ) [static], [private]

return the next available interface ID for no-ID user methods

Rationale: The parser allows multiple user-specified interfaces with empty (unspecified) ID. However, only a single Interface with empty ID can be constructed (if it's the only one present, or the "last one parsed"). Therefore decided to prefer NO_ID over NO_ID_<num> for consistency with interface NO_ID convention. Additionally, NO_ID is preferred over NO_INTERFACE_ID (contrast with Iterator and Model) to preserve backward compatibility

Referenced by Interface::Interface().

14.94.3.7 String no_spec_id ( ) [static], [private]

return the next available interface ID for on-the-fly methods

Rationale: For now NOSPEC_ID_ is chosen due to historical id="NO_SPECIFICATION" used for internally-constructed Iterators. Longer-term, consider auto-generating an ID that includes the context from which the method is constructed, e.g., the parent method or model's ID, together with its name.

References Interface::noSpecIdNum.

14.94.4 Member Data Documentation

14.94.4.1 IntResponseMap rawResponseMap [protected]

Set of responses returned by either a blocking or nonblocking schedule.

The map is a full/partial set of completions which are identified through their evalIdCntr key. The raw set is postprocessed (i.e., finite diff grads merged) in Model::synchronize() where it becomes responseMap.

Referenced by ApplicationInterface::asynchronous_local_evaluations(), Interface::cache_unmatched_response(), Interface::cache_unmatched_responses(), ApplicationInterface::process_asynch_local(), ApplicationInterface::process_synch_local(), ApplicationInterface::receive_evaluation(), Interface::response_map(), ApplicationInterface::synchronize(), ApproximationInterface::synchronize(), ApplicationInterface::synchronize_nowait(), ApproximationInterface::synchronize_nowait(), ApplicationInterface::test_local_backfill(), and ApplicationInterface::test_receives_backfill().

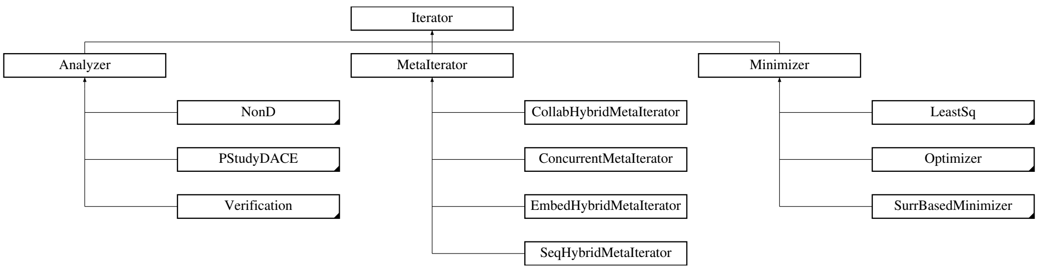
The documentation for this class was generated from the following files:

- DakotaInterface.hpp
- DakotaInterface.cpp

14.95 Iterator Class Reference

Base class for the iterator class hierarchy.

Inheritance diagram for Iterator:



Public Member Functions

- Iterator (std::shared_ptr< TraitsBase > traits=std::shared_ptr< TraitsBase >(new TraitsBase()))

  default constructor
- Iterator (ProblemDescDB &problem_db, std::shared_ptr< TraitsBase > traits=std::shared_ptr< TraitsBase >(new TraitsBase()))

  standard envelope constructor, which constructs its own model(s)
- Iterator (ProblemDescDB &problem_db, Model &model, std::shared_ptr< TraitsBase > traits=std::shared_-ptr< TraitsBase >(new TraitsBase()))

  alternate envelope constructor which uses the ProblemDescDB but accepts a model from a higher level (meta-iterator) context, instead of constructing its own
- Iterator (const String &method_string, Model &model, std::shared_ptr< TraitsBase > traits=std::shared_ptr< TraitsBase >(new TraitsBase()))

alternate envelope constructor for instantiations by name without the ProblemDescDB

- Iterator (const Iterator &iterator)

  copy constructor
- virtual ∼Iterator ()

  destructor
- Iterator operator= (const Iterator &iterator)

  assignment operator
- virtual void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- virtual void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- virtual void initialize_run ()

  utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
- virtual void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- virtual void core_run ()

  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- virtual void post_run (std::ostream &s)

  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- virtual void finalize_run ()

  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
- virtual void pre_output ()

  write variables to file, following pre-run
- virtual void post_input ()

  read tabular data for post-run mode
- virtual void reset ()

  restore initial state for repeated sub-iterator executions
- virtual void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_-target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

  set primaryA{CV,DIV,DRV}MapIndices, secondaryA{CV,DIV,DRV}MapTargets within derived Iterators; supports computation of higher-level sensitivities in nested contexts (e.g., derivatives of statistics w.r.t. inserted design variables)
- virtual void nested_response_mappings (const RealMatrix &primary_coeffs, const RealMatrix &secondary_-coeffs)

  set primaryResponseCoefficients, secondaryResponseCoefficients within derived Iterators; Necessary for scalarization case in MLMC NonDMultilevelSampling to map scalarization in nested context
- virtual void initialize_iterator (int job_index)

  used by IteratorScheduler to set the starting data for a run
- virtual void pack_parameters_buffer (MPIPackBuffer &send_buffer, int job_index)

  used by IteratorScheduler to pack starting data for an iterator run
- virtual void unpack_parameters_buffer (MPIUnpackBuffer &recv_buffer, int job_index)

  used by IteratorScheduler to unpack starting data for an iterator run
- virtual void unpack_parameters_initialize (MPIUnpackBuffer &recv_buffer, int job_index)

  used by IteratorScheduler to unpack starting data and initialize an iterator run
- virtual void pack_results_buffer (MPIPackBuffer &send_buffer, int job_index)

  used by IteratorScheduler to pack results data from an iterator run
- virtual void unpack_results_buffer (MPIUnpackBuffer &recv_buffer, int job_index)

  used by IteratorScheduler to unpack results data from an iterator run
- virtual void update_local_results (int job_index)

used by IteratorScheduler to update local results arrays

- virtual const Variables & variables_results () const

  return a single final iterator solution (variables)
- virtual const Response & response_results () const

  return a single final iterator solution (response)
- virtual const VariablesArray & variables_array_results ()

  return multiple final iterator solutions (variables). This should only be used if returns_multiple_points() returns true.
- virtual const ResponseArray & response_array_results ()

  return multiple final iterator solutions (response). This should only be used if returns_multiple_points() returns true.
- virtual void response_results_active_set (const ActiveSet &set)

  set the requested data for the final iterator response results
- virtual const RealSymMatrix & response_error_estimates () const

  return error estimates associated with the final iterator solution
- virtual bool accepts_multiple_points () const

  indicates if this iterator accepts multiple initial points. Default return is false. Override to return true if appropriate.
- virtual bool returns_multiple_points () const

  indicates if this iterator returns multiple final points. Default return is false. Override to return true if appropriate.
- virtual void initial_point (const Variables &pt)

  sets the initial point for this iterator (user-functions mode for which Model updating is not used)
- virtual void initial_point (const RealVector &pt)

  sets the initial point (active continuous variables) for this iterator (user-functions mode for which Model updating is not used)
- virtual void initial_points (const VariablesArray &pts)

  sets the multiple initial points for this iterator. This should only be used if accepts_multiple_points() returns true.
- virtual void variable_bounds (const RealVector &cv_lower_bnds, const RealVector &cv_upper_bnds)

  assign nonlinear inequality and equality constraint allowables for this iterator (user-functions mode for which Model updating is not used)
- virtual void linear_constraints (const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_lb, const RealVector &lin_ineq_ub, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_tgt)

  assign linear inequality and linear equality constraints for this iterator (user-functions mode for which Model updating is not used)
- virtual void nonlinear_constraints (const RealVector &nln_ineq_lb, const RealVector &nln_ineq_ub, const RealVector &nln_eq_tgt)

  assign nonlinear inequality and equality constraint allowables for this iterator (user-functions mode for which Model updating is not used)
- virtual void initialize_graphics (int iterator_server_id=1)

  initialize the 2D graphics window and the tabular graphics data
- virtual void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final iterator results
- virtual const Model & algorithm_space_model () const

  return the result of any recasting or surrogate model recursion layered on top of iteratedModel by the derived Iterator ctor chain
- virtual void check_sub_iterator_conflict ()

  detect any conflicts due to recursive use of the same Fortran solver
- virtual unsigned short uses_method () const

  return name of any enabling iterator used by this iterator
- virtual void method_recourse ()

  perform a method switch, if possible, due to a detected conflict
- virtual const VariablesArray & all_variables ()

  return the complete set of evaluated variables
- virtual const RealMatrix & all_samples ()

  return the complete set of evaluated samples

- virtual const IntResponseMap & all_responses () const

  return the complete set of computed responses
- virtual size_t num_samples () const

  get the current number of samples
- virtual void sampling_reset (size_t min_samples, bool all_data_flag, bool stats_flag)

  reset sampling iterator to use at least min_samples
- virtual void sampling_reference (size_t samples_ref)

  set reference number of samples, which is a lower bound during reset
- virtual void sampling_increment ()

  increment to next in sequence of refinement samples
- virtual void random_seed (int seed)

  set randomSeed, if present
- virtual unsigned short sampling_scheme () const

  return sampling name
- virtual bool compact_mode () const

  returns Analyzer::compactMode
- virtual IntIntPair estimate_partition_bounds ()

  estimate the minimum and maximum partition sizes that can be utilized by this Iterator
- virtual bool resize ()

  reinitializes iterator based on new variable size
- virtual void declare_sources ()

  Declare sources to the evaluations database.
- void init_communicators (ParLevLIter pl_iter)

  initialize the communicators associated with this Iterator instance
- void set_communicators (ParLevLIter pl_iter)

  set the communicators associated with this Iterator instance
- void free_communicators (ParLevLIter pl_iter)

  free the communicators associated with this Iterator instance
- void resize_communicators (ParLevLIter pl_iter, bool reinit_comms)

  Resize the communicators. This is called from the letter's resize()
- void parallel_configuration_iterator (ParConfigLIter pc_iter)

  set methodPCIter
- ParConfigLIter parallel_configuration_iterator () const

  return methodPCIter
- void parallel_configuration_iterator_map (std::map< size_t, ParConfigLIter > pci_map)

  set methodPCIterMap
- std::map< size_t, ParConfigLIter > parallel_configuration_iterator_map () const

  return methodPCIterMap
- void run (ParLevLIter pl_iter)

  invoke set_communicators(pl_iter) prior to run()
- void run ()

  orchestrate initialize/pre/core/post/finalize phases
- void assign_rep (std::shared_ptr< Iterator > iterator_rep)

  replaces existing letter with a new one
- void iterated_model (const Model &model)

  set the iteratedModel (iterators and meta-iterators using a single model instance)
- Model & iterated_model ()

  return the iteratedModel (iterators & meta-iterators using a single model instance)
- ProblemDescDB & problem_description_db () const

  return the problem description database (probDescDB)
- ParallelLibrary & parallel_library () const

return the parallel library (parallelLib)

- void method_name (unsigned short m_name)

  set the method name to an enumeration value
- unsigned short method_name () const

  return the method name via its native enumeration value
- void method_string (const String &m_str)

  set the method name by string
- String method_string () const

  return the method name by string
- String method_enum_to_string (unsigned short method_enum) const

  convert a method name enumeration value to a string
- unsigned short method_string_to_enum (const String &method_str) const

  convert a method name string to an enumeration value
- String submethod_enum_to_string (unsigned short submethod_enum) const

  convert a sub-method name enumeration value to a string
- const String & method_id () const

  return the method identifier (methodId)
- int maximum_evaluation_concurrency () const

  return the maximum evaluation concurrency supported by the iterator
- void maximum_evaluation_concurrency (int max_conc)

  set the maximum evaluation concurrency supported by the iterator
- size_t maximum_iterations () const

  return the maximum iterations for this iterator
- void maximum_iterations (size_t max_iter)

  set the maximum iterations for this iterator
- void convergence_tolerance (Real conv_tol)

  set the method convergence tolerance (convergenceTol)
- Real convergence_tolerance () const

  return the method convergence tolerance (convergenceTol)
- void output_level (short out_lev)

  set the method output level (outputLevel)
- short output_level () const

  return the method output level (outputLevel)
- void summary_output (bool summary_output_flag)

  Set summary output control; true enables evaluation/results summary.
- size_t num_final_solutions () const

  return the number of solutions to retain in best variables/response arrays
- void num_final_solutions (size_t num_final)

  set the number of solutions to retain in best variables/response arrays
- void active_set (const ActiveSet &set)

  set the default active set (for use with iterators that employ evaluate_parameter_sets())
- const ActiveSet & active_set () const

  return the default active set (used by iterators that employ evaluate_parameter_sets())
- void active_set_request_vector (const ShortArray &asv)

  return the default active set request vector (used by iterators that employ evaluate_parameter_sets())
- const ShortArray & active_set_request_vector () const

  return the default active set request vector (used by iterators that employ evaluate_parameter_sets())
- void active_set_request_values (short asv_val)

  return the default active set request vector (used by iterators that employ evaluate_parameter_sets())
- void sub_iterator_flag (bool si_flag)

  set subIteratorFlag (and update summaryOutputFlag if needed)

- bool is_null () const

  function to check iteratorRep (does this envelope contain a letter?)
- std::shared_ptr< Iterator > iterator_rep () const

  returns iteratorRep for access to derived class member functions that are not mapped to the top Iterator level
- virtual void eval_tag_prefix (const String &eval_id_str)

  set the hierarchical eval ID tag prefix
- std::shared_ptr< TraitsBase > traits () const

  returns methodTraits for access to derived class member functions that are not mapped to the top TraitsBase level
- bool top_level ()

  Return whether the iterator is the top level iterator.
- void top_level (bool tflag)

  Set the iterator's top level flag.

Protected Member Functions

- Iterator (BaseConstructor, ProblemDescDB &problem_db, std::shared_ptr< TraitsBase > traits=std::shared-_ptr< TraitsBase >(new TraitsBase()))

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- Iterator (NoDBBaseConstructor, unsigned short method_name, Model &model, std::shared_ptr< TraitsBase > traits=std::shared_ptr< TraitsBase >(new TraitsBase()))

  alternate constructor for base iterator classes constructed on the fly
- Iterator (NoDBBaseConstructor, unsigned short method_name, std::shared_ptr< TraitsBase > traits=std-::shared_ptr< TraitsBase >(new TraitsBase()))

  alternate constructor for base iterator classes constructed on the fly
- Iterator (NoDBBaseConstructor, Model &model, size_t max_iter, size_t max_eval, Real conv_tol, std::shared-_ptr< TraitsBase > traits=std::shared_ptr< TraitsBase >(new TraitsBase()))

  alternate envelope constructor for instantiations without ProblemDescDB
- virtual void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- virtual void update_from_model (const Model &model)

  set inherited data attributes based on extractions from incoming model
- virtual const VariablesArray & initial_points () const

  gets the multiple initial points for this iterator. This will only be meaningful after a call to initial_points mutator.
- StrStrSizet run_identifier () const

  get the unique run identifier based on method name, id, and number of executions
- void initialize_model_graphics (Model &model, int iterator_server_id)

  helper function that encapsulates initialization operations, modular on incoming Model instance
- void export_final_surrogates (Model &data_fit_surr_model)

  export final surrogates generated, e.g., GP in EGO and friends

Static Protected Member Functions

- static void gnewton_set_recast (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub-_model_set)

  conversion of request vector values for the Gauss-Newton Hessian approximation

Protected Attributes

- ProblemDescDB & probDescDB

  class member reference to the problem description database
- ParallelLibrary & parallelLib

  class member reference to the parallel library
- ParConfigLIter methodPCIter

  the active ParallelConfiguration used by this Iterator instance
- Model iteratedModel

  the model to be iterated (for iterators and meta-iterators employing a single model instance)
- size_t myModelLayers

  number of Models locally (in Iterator or derived classes) wrapped around the initially passed in Model
- unsigned short methodName

  name of the iterator (the user's method spec)
- Real convergenceTol

  iteration convergence tolerance
- size_t maxIterations

  maximum number of iterations for the method
- size_t maxFunctionEvals

  maximum number of fn evaluations for the method
- int maxEvalConcurrency

  maximum number of concurrent model evaluations
- ActiveSet activeSet

  the response data requirements on each function evaluation
- size_t numFinalSolutions

  number of solutions to retain in best variables/response arrays
- VariablesArray bestVariablesArray

  collection of N best solution variables found during the study; always in context of Model originally passed to the Iterator (any in-flight Recasts must be undone)
- ResponseArray bestResponseArray

  collection of N best solution responses found during the study; always in context of Model originally passed to the Iterator (any in-flight Recasts must be undone)
- bool subIteratorFlag

  flag indicating if this Iterator is a sub-iterator (NestedModel::subIterator or DataFitSurrModel::daceIterator)
- short outputLevel

  output verbosity level: {SILENT,QUIET,NORMAL,VERBOSE,DEBUG}_OUTPUT
- bool summaryOutputFlag

  flag for summary output (evaluation stats, final results); default true, but false for on-the-fly (helper) iterators and sub-iterator use cases
- ResultsManager & resultsDB

  reference to the global iterator results database
- EvaluationStore & evaluationsDB

  reference to the global evaluation database
- EvaluationsDBState evaluationsDBState

  State of evaluations DB for this iterator.
- ResultsNames resultsNames

  valid names for iterator results
- std::shared_ptr< TraitsBase > methodTraits

  pointer that retains shared ownership of a TraitsBase object, or child thereof
- bool topLevel

  Whether this is the top level iterator.
- bool exportSurrogate = false

whether to export final surrogates
- String surrExportPrefix

  base filename for exported surrogates
- unsigned short surrExportFormat = NO_MODEL_FORMAT

  (bitwise) format(s) to export

Private Member Functions

- std::shared_ptr< Iterator > get_iterator (ProblemDescDB &problem_db)

  Used by the envelope to instantiate the correct letter class.
- std::shared_ptr< Iterator > get_iterator (ProblemDescDB &problem_db, Model &model)

  Used by the envelope to instantiate the correct letter class.
- std::shared_ptr< Iterator > get_iterator (const String &method_string, Model &model)

  Used by the envelope to instantiate the correct letter class.

Static Private Member Functions

- static String user_auto_id ()

  return the next available method ID for no-ID user methods
- static String no_spec_id ()

  return the next available method ID for on-the-fly methods

Private Attributes

- String methodId

  method identifier string from the input file, or an auto-generated ID, such that each instance of an Iterator has a unique ID
- size_t execNum

  An execution number for this instance of the class. Now that each instance has a unique methodId, this is just a simple counter.
- std::map< size_t, ParConfigLIter > methodPCIterMap

  track the available configurations that have been created (init_communicators) and are available for activation at run time (set_communicators)
- std::shared_ptr< Iterator > iteratorRep

  pointer to the letter (initialized only for the envelope)

Static Private Attributes

- static size_t noSpecIdNum = 0

  the last used method ID number for on-the-fly instantiations (increment before each use)

14.95.1 Detailed Description

Base class for the iterator class hierarchy.

The Iterator class is the base class for one of the primary class hierarchies in DAKOTA. The iterator hierarchy contains all of the iterative algorithms which use repeated execution of simulations as function evaluations. For memory efficiency and enhanced polymorphism, the iterator hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Iterator) serves as the envelope and one of the derived classes (selected in Iterator::get_iterator()) serves as the letter.

14.95.2 Constructor & Destructor Documentation

14.95.2.1 Iterator (std::shared_ptr< TraitsBase > *traits* = std::shared_ptr<TraitsBase>(new TraitsBase()))

default constructor

The default constructor is used in Vector<Iterator> instantiations and for initialization of Iterator objects contained in meta-Iterators and Model recursions. iteratorRep is NULL in this case.

14.95.2.2 Iterator (ProblemDescDB & *problem_db*, std::shared_ptr< TraitsBase > *traits* = std::shared_ptr<TraitsBase>(new TraitsBase()))

standard envelope constructor, which constructs its own model(s)

This constructor assigns a representation pointer into this envelope, transferring ownership. It behaves the same as a default construction followed by assign_rep(). Envelope constructor only needs to extract enough data to properly execute get_iterator(), since letter holds the actual base class data. This version is used for top-level ProblemDescDB-driven construction of all Iterators and MetaIterators, which construct their own Model instances.

References Dakota::abort_handler(), and Iterator::iteratorRep.

14.95.2.3 Iterator (ProblemDescDB & *problem_db*, Model & *model*, std::shared_ptr< TraitsBase > *traits* = std::shared_ptr<TraitsBase>(new TraitsBase()))

alternate envelope constructor which uses the ProblemDescDB but accepts a model from a higher level (meta-iterator) context, instead of constructing its own

Envelope constructor only needs to extract enough data to properly execute get_iterator(), since letter holds the actual base class data. This version is used for ProblemDescDB-driven construction of Iterators that are passed a Model from a higher-level context (e.g., a MetaIterator instantiates its sub-iterator(s) by name instead of pointer and passes in its iteratedModel, since these sub-iterators lack their own model pointers).

References Dakota::abort_handler(), and Iterator::iteratorRep.

14.95.2.4 Iterator (const String & *method_string*, Model & *model*, std::shared_ptr< TraitsBase > *traits* = std::shared_ptr<TraitsBase>(new TraitsBase()))

alternate envelope constructor for instantiations by name without the ProblemDescDB

Used in sub-iterator instantiations within iterator constructors. Envelope constructor only needs to extract enough data to properly execute get_iterator(), since letter holds the actual base class data. This version is used for lightweight constructions without the ProblemDescDB.

References Dakota::abort_handler(), and Iterator::iteratorRep.

14.95.2.5 Iterator (const Iterator & *iterator*)

copy constructor

Copy constructor manages sharing of iteratorRep.

14.95.2.6 Iterator (BaseConstructor , ProblemDescDB & *problem_db*, std::shared_ptr< TraitsBase > *traits* = std::shared_ptr<TraitsBase>(new TraitsBase())) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor builds the base class data for all inherited iterators, including meta-iterators. get_iterator() instantiates a derived class and the derived class selects this base class constructor in its initialization list (to avoid the recursion of the base class constructor calling get_iterator() again). Since the letter IS the representation, its representation pointer is set to NULL

References Iterator::method_enum_to_string(), Iterator::methodId, Iterator::methodName, Iterator::outputLevel, and Iterator::user_auto_id().

14.95.2.7 Iterator (NoDBBaseConstructor , unsigned short *method_name*, Model & *model*, std::shared_ptr< TraitsBase > *traits* = `std::shared_ptr<TraitsBase>(new TraitsBase())`) `[protected]`

alternate constructor for base iterator classes constructed on the fly

This alternate constructor builds base class data for inherited iterators. It is used for on-the-fly instantiations for which DB queries cannot be used, and is not used for construction of meta-iterators.

14.95.2.8 Iterator (NoDBBaseConstructor , unsigned short *method_name*, std::shared_ptr< TraitsBase > *traits* = `std::shared_ptr<TraitsBase>(new TraitsBase())`) `[protected]`

alternate constructor for base iterator classes constructed on the fly

This alternate constructor builds base class data for inherited iterators. It is used for on-the-fly instantiations for which DB queries cannot be used, and is not used for construction of meta-iterators. It has no incoming model, so only sets up a minimal set of defaults. However, its use is preferable to the default constructor, which should remain as minimal as possible.

14.95.2.9 Iterator (NoDBBaseConstructor , Model & *model*, size_t *max_iter*, size_t *max_eval*, Real *conv_tol*, std::shared_ptr< TraitsBase > *traits* = `std::shared_ptr<TraitsBase>(new TraitsBase())`) `[protected]`

alternate envelope constructor for instantiations without ProblemDescDB

This alternate constructor builds base class data for inherited iterators. It is used for on-the-fly instantiations for which DB queries cannot be used, and is not used for construction of meta-iterators.

14.95.3 Member Function Documentation

14.95.3.1 void initialize_run ( ) `[virtual]`

utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers

Perform initialization phases of run sequence, like allocating memory and setting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's initialize_run(), typically *before* performing its own implementation steps.

Reimplemented in Optimizer, SNLLOptimizer, APPSOptimizer, SNLLLeastSq, Minimizer, CONMINOptimizer, Analyzer, NonD, ROLOptimizer, and LeastSq.

References Iterator::iteratorRep.

Referenced by Iterator::run(), and SeqHybridMetaIterator::run_sequential_adaptive().

14.95.3.2 void pre_run ( ) `[virtual]`

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented in NonDSampling, Analyzer, NonDBayesCalibration, NonDLHSSampling, EffGlobalMinimizer, NonDLocalReliability, NonDNonHierarchSampling, DDACEDesignCompExp, ConcurrentMetaIterator, NonDRKDDarts, NonDEnsembleSampling, SurrBasedLocalMinimizer, FSUDesignCompExp, ParamStudy, PSUADEDesignCompExp, NonDGlobalReliability, and NonDMultilevControlVarSampling.

References Iterator::iteratorRep.

Referenced by NonDBayesCalibration::build_designs(), and Iterator::run().

14.95.3.3 void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented in JEGAOptimizer, NonDSampling, NOWPACOptimizer, SNLLOptimizer, APPSOptimizer, COLINOptimizer, SNLLLeastSq, NonDIntegration, CONMINOptimizer, NLSSOLLeastSq, SurrBasedGlobalMinimizer, NonDBayesCalibration, NonDLHSSampling, EffGlobalMinimizer, NCSUOptimizer, NonDMultilevelPolynomialChaos, NonlinearCGOptimizer, ROLOptimizer, NL2SOLLeastSq, NonDLocalReliability, NonDMultilevelFunctionTrain, OptDartsOptimizer, NonDAdaptImpSampling, SeqHybridMetaIterator, NonDAdaptiveSampling, ConcurrentMetaIterator, DDACEDesignCompExp, NonDExpansion, SurrBasedLocalMinimizer, NonDGPImpSampling, NonDMultilevelStochCollocation, NonDPOFDarts, FSUDesignCompExp, NonDACVSampling, NonDGlobalInterval, NonDLocalInterval, NonDMultifidelitySampling, ParamStudy, PSUADEDesignCompExp, EmbedHybridMetaIterator, NonDGlobalReliability, NonDMultilevelSampling, CollabHybridMetaIterator, NonDMultilevControlVarSampling, NonDLHSInterval, NonDControlVariateSampling, NonDRKDDarts, and RichExtrapVerification.

References Dakota::abort_handler(), and Iterator::iteratorRep.

Referenced by Iterator::run().

14.95.3.4 void post_run (std::ostream & *s*) [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented in Optimizer, SNLLOptimizer, COLINOptimizer, Minimizer, NonDRKDDarts, Analyzer, NonDLHSSampling, EffGlobalMinimizer, DDACEDesignCompExp, SurrBasedLocalMinimizer, NonDEnsembleSampling, FSUDesignCompExp, MetaIterator, NonDReliability, ParamStudy, PSUADEDesignCompExp, and LeastSq.

References Iterator::iteratorRep.

Referenced by Iterator::run().

14.95.3.5 void finalize_run ( ) [virtual]

utility function to perform common operations following post_run(); deallocation and resetting of instance pointers

Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's finalize_run(), typically *after* performing its own implementation steps.

Reimplemented in Optimizer, SNLLOptimizer, SNLLLeastSq, Minimizer, Analyzer, NonD, and LeastSq.

References Iterator::iteratorRep.

Referenced by Iterator::run(), and SeqHybridMetaIterator::run_sequential_adaptive().

14.95.3.6 void initialize_graphics (int *iterator_server_id* = 1) [virtual]

initialize the 2D graphics window and the tabular graphics data

This is a convenience function for encapsulating graphics initialization operations. It is overridden by derived classes that specialize the graphics display.

Reimplemented in SurrBasedGlobalMinimizer, NonDLocalReliability, and SurrBasedLocalMinimizer.

References Iterator::initialize_model_graphics(), Iterator::iteratedModel, and Iterator::iteratorRep.

Referenced by CollabHybridMetaIterator::core_run(), EmbedHybridMetaIterator::core_run(), ConcurrentMetaIterator::core_run(), Environment::execute(), SeqHybridMetaIterator::run_sequential(), and SeqHybridMetaIterator::run_sequential_adaptive().

14.95.3.7 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented in Optimizer, NonDPolynomialChaos, Analyzer, NonDGPMSABayesCalibration, NonDLHSSampling, NonDMultilevelPolynomialChaos, NonDBayesCalibration, NonDMultilevelFunctionTrain, NonDPOFDarts, NonDQUESOBayesCalibration, NonDMultilevelStochCollocation, NonDAdaptImpSampling, NonDLocalReliability, NonDWASABIBayesCalibration, SeqHybridMetaIterator, NonDAdaptiveSampling, ConcurrentMetaIterator, NonDExpansion, NonDGPImpSampling, NonDMUQBayesCalibration, NonDEnsembleSampling, NonDInterval, PStudyDACE, SurrBasedMinimizer, NonDGlobalReliability, LeastSq, Verification, and RichExtrapVerification.

References Iterator::iteratorRep.

Referenced by MetaIterator::post_run(), and Minimizer::post_run().

14.95.3.8 void check_sub_iterator_conflict ( ) [virtual]

detect any conflicts due to recursive use of the same Fortran solver

This is used to avoid clashes in state between non-object-oriented (i.e., F77, C) iterator executions, when such iterators could potentially be executing simultaneously (e.g., nested execution). It is not an issue (and a used method is not reported) in cases where a helper execution is completed before a lower level one could be initiated; an example of this is DIRECT for maximization of expected improvement: the EIF maximization is completed before a new point evaluation (which could include nested iteration) is performed.

Reimplemented in CONMINOptimizer, NLSSOLLeastSq, NCSUOptimizer, NonDLocalReliability, and NonDLocalInterval.

References Iterator::iteratorRep.

Referenced by Iterator::init_communicators().

14.95.3.9 void run ( )

orchestrate initialize/pre/core/post/finalize phases

Iterator supports a construct/initialize-run/pre-run/core-run/post-run/ finalize-run/destruct progression. This member (non-virtual) function sequences these run phases.

References ParallelLibrary::command_line_post_run(), ParallelLibrary::command_line_pre_run(), ParallelLibrary::command_line_run(), Iterator::core_run(), Iterator::declare_sources(), Iterator::evaluationsDB, Iterator::evaluationsDBState, Iterator::execNum, Iterator::finalize_run(), ResultsManager::flush(), Iterator::initialize_run(), Iterator::iteratorRep, Iterator::method_enum_to_string(), Iterator::method_id(), Iterator::method_string(), Iterator-

::methodName, Iterator::outputLevel, Iterator::parallelLib, Iterator::post_input(), Iterator::post_run(), Iterator::pre_-output(), Iterator::pre_run(), Iterator::resultsDB, Iterator::summaryOutputFlag, and Iterator::top_level().

Referenced by Iterator::run().

14.95.3.10 void assign_rep (std::shared_ptr< Iterator > *iterator_rep*)

replaces existing letter with a new one

The assign_rep() function is used for publishing derived class letters to existing envelopes, as opposed to sharing representations among multiple envelopes (in particular, assign_rep is passed a letter object and operator= is passed an envelope object).

Use case assumes the incoming letter is instantiated on the fly and has no envelope. This case is modeled after get_iterator(): a letter is dynamically allocated and passed into assign_rep (its memory management is passed over to the envelope).

If the letter happens to be managed by another envelope, it will persist as long as the last envelope referencing it.

References Iterator::iterator_rep(), and Iterator::iteratorRep.

Referenced by AdaptedBasisModel::AdaptedBasisModel(), NonDBayesCalibration::build_designs(), NonD-Expansion::construct_cubature(), NonDExpansion::construct_expansion_sampler(), NonDAdaptiveSampling-::construct_fsu_sampler(), NonD::construct_lhs(), NonDBayesCalibration::construct_map_optimizer(), NonD-BayesCalibration::construct_mcmc_model(), NonDExpansion::construct_quadrature(), NonDExpansion::construct-_sparse_grid(), Minimizer::data_transform_model(), ActiveSubspaceModel::init_fullspace_sampler(), EffGlobal-Minimizer::initialize_sub_problem(), NonDLocalInterval::method_recourse(), NonDLocalReliability::method_-recourse(), NonDAdaptiveSampling::NonDAdaptiveSampling(), NonDBayesCalibration::NonDBayesCalibration(), NonDGlobalInterval::NonDGlobalInterval(), NonDGlobalReliability::NonDGlobalReliability(), NonDGPImpSampling-::NonDGPImpSampling(), NonDGPMSABayesCalibration::NonDGPMSABayesCalibration(), NonDLHSInterval::-NonDLHSInterval(), NonDLocalInterval::NonDLocalInterval(), NonDLocalReliability::NonDLocalReliability(), Gauss-ProcApproximation::optimize_theta_global(), GaussProcApproximation::optimize_theta_multipoint(), and Surr-BasedLocalMinimizer::relax_constraints().

14.95.3.11 void eval_tag_prefix (const String & *eval_id_str*) [virtual]

set the hierarchical eval ID tag prefix

This prepend may need to become a virtual function if the tagging should propagate to other subModels or helper Iterators an Iterator may contain.

References Model::eval_tag_prefix(), Iterator::iteratedModel, and Iterator::iteratorRep.

Referenced by NestedModel::derived_evaluate(), Iterator::init_communicators(), NestedModel::initialize_iterator(), and DataFitSurrModel::run_dace().

14.95.3.12 void gnewton_set_recast (const Variables & *recast_vars*, const ActiveSet & *recast_set*, ActiveSet & *sub_model_set*) [static], [protected]

conversion of request vector values for the Gauss-Newton Hessian approximation

For Gauss-Newton Hessian requests, activate the 2 bit and mask the 4 bit.

References ActiveSet::request_value(), and ActiveSet::request_vector().

Referenced by NonDBayesCalibration::construct_map_model(), and Optimizer::reduce_model().

14.95.3.13 void initialize_model_graphics (Model & *model*, int *iterator_server_id*) [protected]

helper function that encapsulates initialization operations, modular on incoming Model instance

This is a helper function that provides modularity on incoming Model.

References Model::auto_graphics(), Model::create_2d_plots(), Model::create_tabular_datastream(), OutputManager::graph2DFlag, ParallelLibrary::output_manager(), Iterator::parallelLib, and OutputManager::tabularDataFlag.

Referenced by SurrBasedGlobalMinimizer::initialize_graphics(), and Iterator::initialize_graphics().

14.95.3.14 void export_final_surrogates (**Model** & *data_fit_surr_model*) [protected]

export final surrogates generated, e.g., GP in EGO and friends

Protected function to only be called on letters

References Dakota::abort_handler(), Model::approximations(), Model::current_variables(), Iterator::exportSurrogate, Model::response_labels(), Iterator::surrExportFormat, and Iterator::surrExportPrefix.

Referenced by NonDGlobalInterval::core_run(), NonDGlobalReliability::optimize_gaussian_process(), and EffGlobalMinimizer::retrieve_final_results().

14.95.3.15 std::shared_ptr< **Iterator** > get_iterator (**ProblemDescDB** & *problem_db*) [private]

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize iteratorRep to the appropriate derived type, as given by the DB's method_name. Supports all iterators and meta-iterators. These instantiations will NOT recurse on the Iterator(problem_db) constructor due to the use of BaseConstructor.

References ProblemDescDB::get_model(), ProblemDescDB::get_ushort(), Iterator::method_name(), and Dakota::SUBMETHOD_COLLABORATIVE.

14.95.3.16 std::shared_ptr< **Iterator** > get_iterator (**ProblemDescDB** & *problem_db,* **Model** & *model*) [private]

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize iteratorRep to the appropriate derived type. Alternate construction of meta-iterators is supported to enable use of meta-iterators as components. These instantiations will NOT recurse on the Iterator(problem_db, model) constructor due to the use of BaseConstructor.

References ProblemDescDB::get_ushort(), Iterator::method_enum_to_string(), Iterator::method_name(), Iterator::probDescDB, Dakota::SUBMETHOD_COLLABORATIVE, Iterator::submethod_enum_to_string(), and Model::surrogate_type().

14.95.3.17 std::shared_ptr< **Iterator** > get_iterator (const String & *method_string,* **Model** & *model*) [private]

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize iteratorRep to the appropriate derived type, as given by the passed method_string. Lightweight instantiations by name are supported by a subset of Iterators (primarily Minimizers).

References Iterator::method_string(), Dakota::strbegins(), and Dakota::strends().

14.95.3.18 String user_auto_id ( ) [static], [private]

return the next available method ID for no-ID user methods

Rationale: The parser allows multiple user-specified methods with empty (unspecified) ID. However, only a single Iterator with empty ID can be constructed (if it's the only one present, or the "last one parsed"). Therefore decided to prefer NO_METHOD_ID over NO_METHOD_ID_<num> for (partial) consistency with interface NO_ID convention. The addition of *METHOD* is it distinguish methods, models and interfaces in the HDF5 output.

Referenced by Iterator::Iterator().

14.95.3.19 String no_spec_id ( ) [static], [private]

return the next available method ID for on-the-fly methods

Rationale: For now NOSPEC_METHOD_ID_ is chosen due to historical id="NO_SPECIFICATION" used for internally-constructed Iterators. Longer-term, consider auto-generating an ID that includes the context from which the method is constructed, e.g., the parent method or model's ID, together with its name.

References Iterator::noSpecIdNum.

14.95.4 Member Data Documentation

14.95.4.1 ProblemDescDB& probDescDB [protected]

class member reference to the problem description database

Iterator and Model cannot use a shallow copy of ProblemDescDB due to circular destruction dependency (reference counts can't get to 0), since ProblemDescDB contains {iterator,model}List.

Referenced by MetaIterator::allocate_by_name(), MetaIterator::allocate_by_pointer(), Analyzer::Analyzer(), MetaIterator::check_model(), COLINOptimizer::COLINOptimizer(), NonDC3FunctionTrain::config_regression(), NonDBayesCalibration::construct_mcmc_model(), Minimizer::data_transform_model(), SurrBasedMinimizer::derived_init_communicators(), EmbedHybridMetaIterator::derived_init_communicators(), ConcurrentMetaIterator::derived_init_communicators(), EffGlobalMinimizer::EffGlobalMinimizer(), MetaIterator::estimate_by_name(), MetaIterator::estimate_by_pointer(), CollabHybridMetaIterator::estimate_partition_bounds(), EmbedHybridMetaIterator::estimate_partition_bounds(), ConcurrentMetaIterator::estimate_partition_bounds(), SeqHybridMetaIterator::estimate_partition_bounds(), FSUDesignCompExp::FSUDesignCompExp(), Optimizer::get_common_-stopping_criteria(), Iterator::get_iterator(), NonDC3FunctionTrain::initialize_c3_db_options(), ConcurrentMetaIterator::initialize_model(), NOWPACOptimizer::initialize_options(), SurrBasedLocalMinimizer::initialize_sub_-minimizer(), JEGAOptimizer::JEGAOptimizer(), NLSSOLLeastSq::NLSSOLLeastSq(), NonDAdaptImpSampling::NonDAdaptImpSampling(), NonDAdaptiveSampling::NonDAdaptiveSampling(), NonDBayesCalibration::NonDBayesCalibration(), NonDC3FunctionTrain::NonDC3FunctionTrain(), NonDGlobalInterval::NonDGlobalInterval(), NonDGlobalReliability::NonDGlobalReliability(), NonDGPImpSampling::NonDGPImpSampling(), NonDGPMSABayesCalibration::NonDGPMSABayesCalibration(), NonDInterval::NonDInterval(), NonDLocalInterval::NonDLocalInterval(), NonDLocalReliability::NonDLocalReliability(), NonDMultilevelFunctionTrain::NonDMultilevelFunctionTrain(), NonDMultilevelPolynomialChaos::NonDMultilevelPolynomialChaos(), NonDMultilevelSampling::NonDMultilevelSampling(), NonDMultilevelStochCollocation::NonDMultilevelStochCollocation(), NonDNonHierarchSampling::NonDNonHierarchSampling(), NonDQuadrature::NonDQuadrature(), NonDSampling::NonDSampling(), NonDSparseGrid::NonDSparseGrid(), NonDStochCollocation::NonDStochCollocation(), NonDSurrogateExpansion::NonDSurrogateExpansion(), OptDartsOptimizer::OptDartsOptimizer(), ParamStudy::ParamStudy(), NonlinearCGOptimizer::parse_options(), NonDAdaptiveSampling::parse_options(), Iterator::problem_-description_db(), NonDC3FunctionTrain::resolve_refinement(), APPSOptimizer::set_apps_parameters(), ROLOptimizer::set_rol_parameters(), COLINOptimizer::set_solver_parameters(), SNLLLeastSq::SNLLLeastSq(), SNLLOptimizer::SNLLOptimizer(), COLINOptimizer::solver_setup(), and SurrBasedGlobalMinimizer::SurrBasedGlobalMinimizer().

14.95.4.2 int maxEvalConcurrency [protected]

maximum number of concurrent model evaluations

This is important for parallel configuration init/set/free and may be set within empty envelope instances. Therefore, it cannot be pushed down into Analyzer/Minimizer derived classes.

Referenced by NonDPolynomialChaos::config_expectation(), NonDC3FunctionTrain::config_regression(), NonDPolynomialChaos::config_regression(), DDACEDesignCompExp::DDACEDesignCompExp(), NonDGlobalReliability::derived_free_communicators(), NonDLocalInterval::derived_free_communicators(), NonDGlobalInterval::derived_free_communicators(), NonDExpansion::derived_free_communicators(), SurrBasedMinimizer::derived_free_communicators(), NonDGPImpSampling::derived_free_communicators(), NonDAdaptiveSampling::derived_free_communicators(), NonDLocalReliability::derived_free_communicators(), Iterator::derived_free_communicators(), NonDBayesCalibration::derived_free_communicators(), NonDPolynomialChaos::derived-

_free_communicators(), NonDGlobalReliability::derived_init_communicators(), NonDLocalInterval::derived-_init_communicators(), NonDGlobalInterval::derived_init_communicators(), NonDExpansion::derived_init_-communicators(), SurrBasedMinimizer::derived_init_communicators(), NonDGPImpSampling::derived_init_-communicators(), NonDAdaptiveSampling::derived_init_communicators(), NonDLocalReliability::derived_init_-communicators(), NonDBayesCalibration::derived_init_communicators(), NonDPolynomialChaos::derived_init_-communicators(), Iterator::derived_init_communicators(), NonDExpansion::derived_set_communicators(), Surr-BasedMinimizer::derived_set_communicators(), NonDLocalReliability::derived_set_communicators(), Iterator-::derived_set_communicators(), NonDBayesCalibration::derived_set_communicators(), NonD::derived_set_-communicators(), NonDPolynomialChaos::derived_set_communicators(), Iterator::estimate_partition_bounds(), FSUDesignCompExp::FSUDesignCompExp(), NonDCubature::initialize_grid(), NonDQuadrature::initialize_grid(), NonDSparseGrid::initialize_grid(), EffGlobalMinimizer::initialize_sub_problem(), NonDExpansion::initialize_u-_space_grid(), JEGAOptimizer::JEGAOptimizer(), Iterator::maximum_evaluation_concurrency(), NonDAdapt-ImpSampling::NonDAdaptImpSampling(), NonDBayesCalibration::NonDBayesCalibration(), NonDCubature::-NonDCubature(), NonDGlobalInterval::NonDGlobalInterval(), NonDGlobalReliability::NonDGlobalReliability(), NonDHierarchSampling::NonDHierarchSampling(), NonDLHSInterval::NonDLHSInterval(), NonDNonHierarch-Sampling::NonDNonHierarchSampling(), NonDQuadrature::NonDQuadrature(), NonDSampling::NonDSampling(), NonDSparseGrid::NonDSparseGrid(), Analyzer::num_samples(), ParamStudy::ParamStudy(), PSUADEDesign-CompExp::PSUADEDesignCompExp(), Iterator::resize_communicators(), RichExtrapVerification::RichExtrap-Verification(), APPSOptimizer::set_apps_parameters(), COLINOptimizer::set_solver_parameters(), SNLL-Optimizer::SNLLOptimizer(), and Iterator::update_from_model().

The documentation for this class was generated from the following files:

- DakotaIterator.hpp
- DakotaIterator.cpp

14.96 IteratorScheduler Class Reference

This class encapsulates scheduling operations for concurrent sub-iteration within an outer level context (e.g., meta-iteration, nested models).

Public Member Functions

- IteratorScheduler (ParallelLibrary &parallel_lib, bool peer_assign_jobs, int num_servers=0, int procs_per_-iterator=0, short scheduling=DEFAULT_SCHEDULING)

    constructor
- ∼IteratorScheduler ()

    destructor
- void construct_sub_iterator (ProblemDescDB &problem_db, Iterator &sub_iterator, Model &sub_model, const String &method_ptr, const String &method_name, const String &model_ptr)

    instantiate sub_iterator on the current rank if not already constructed
- IntIntPair configure (ProblemDescDB &problem_db, Iterator &sub_iterator, Model &sub_model)

    performs sufficient initialization to define partitioning controls (min and max processors per iterator server)
- IntIntPair configure (ProblemDescDB &problem_db, const String &method_string, Iterator &sub_iterator, Model &sub_model)

    performs sufficient initialization to define partitioning controls (min and max processors per iterator server)
- IntIntPair configure (ProblemDescDB &problem_db, Iterator &sub_iterator)

    performs sufficient initialization to define partitioning controls (min and max processors per iterator server)
- void partition (int max_iterator_concurrency, IntIntPair &ppi_pr)

    convenience function for initializing iterator communicators, setting parallel configuration attributes, and managing outputs and restart.
- void init_iterator (ProblemDescDB &problem_db, Iterator &sub_iterator, Model &sub_model)

    invokes static version of this function with appropriate parallelism level

- void init_iterator (ProblemDescDB &problem_db, const String &method_string, Iterator &sub_iterator, Model &sub_model)

    invokes static version of this function with appropriate parallelism level
- void set_iterator (Iterator &sub_iterator)

    invokes static version of this function with appropriate parallelism level
- void run_iterator (Iterator &sub_iterator)

    invokes static version of this function with appropriate parallelism level
- void free_iterator (Iterator &sub_iterator)

    invokes static version of this function with appropriate parallelism level
- void free_iterator_parallelism ()

    convenience function for deallocating the concurrent iterator parallelism level
- template<typename MetaType >
  void schedule_iterators (MetaType &meta_object, Iterator &sub_iterator)

    short convenience function for distributing control among master_dynamic_schedule_iterators(), serve_iterators(), and peer_static_schedule_iterators()
- template<typename MetaType >
  void master_dynamic_schedule_iterators (MetaType &meta_object)

    executed by the scheduler master to manage a dynamic schedule of iterator jobs among slave iterator servers
- void stop_iterator_servers ()

    executed by the scheduler master to terminate slave iterator servers
- template<typename MetaType >
  void serve_iterators (MetaType &meta_object, Iterator &sub_iterator)

    executed on the slave iterator servers to perform iterator jobs assigned by the scheduler master
- template<typename MetaType >
  void peer_static_schedule_iterators (MetaType &meta_object, Iterator &sub_iterator)

    executed on iterator peers to manage a static schedule of iterator jobs
- void update (ParConfigLIter pc_iter)

    update schedPCIter
- void update (size_t index)

    update miPLIndex as well as associated settings for concurrent iterator scheduling from the corresponding ParallelLevel
- void update (ParConfigLIter pc_iter, size_t index)

    invoke update(ParConfigLIter) and update(size_t) in sequence
- void iterator_message_lengths (int params_msg_len, int results_msg_len)

    update paramsMsgLen and resultsMsgLen
- bool lead_rank () const

    determines if current processor is rank 0 of the parent comm

Static Public Member Functions

- static void init_iterator (ProblemDescDB &problem_db, Iterator &sub_iterator, ParLevLIter pl_iter)

    convenience function for allocation of an iterator and (parallel) initialization of its comms
- static void init_iterator (ProblemDescDB &problem_db, Iterator &sub_iterator, Model &sub_model, ParLevLIter pl_iter)

    convenience function for allocation of an iterator and (parallel) initialization of its comms
- static void init_iterator (ProblemDescDB &problem_db, const String &method_string, Iterator &sub_iterator, Model &sub_model, ParLevLIter pl_iter)

    convenience function for lightweight allocation of an iterator and (parallel) initialization of its comms
- static void set_iterator (Iterator &sub_iterator, ParLevLIter pl_iter)

    convenience function for setting comms prior to running an iterator
- static void run_iterator (Iterator &sub_iterator, ParLevLIter pl_iter)

Convenience function for invoking an iterator and managing parallelism. This version omits communicator repartitioning. Function must be public due to use by MINLPNode.

- static void free_iterator (Iterator &sub_iterator, ParLevLIter pl_iter)

    convenience function for deallocating comms after running an iterator

Public Attributes

- ParallelLibrary & parallelLib

    reference to the ParallelLibrary instance

- int numIteratorJobs

    number of iterator executions to schedule

- int numIteratorServers

    number of concurrent iterator partitions

- int procsPerIterator

    partition size request

- int iteratorCommRank

    processor rank in iteratorComm

- int iteratorCommSize

    number of processors in iteratorComm

- int iteratorServerId

    identifier for an iterator server

- bool messagePass

    flag for message passing among iterator servers

- short iteratorScheduling

    {DEFAULT,MASTER,PEER}_SCHEDULING

- bool peerAssignJobs

    `flag indicating need for peer 1 to assign jobs`
    < to peers 2-n

- ParConfigLIter schedPCIter

    iterator for active parallel configuration

- size_t miPLIndex

    `index of active parallel level (corresponding`
    < to ParallelConfiguration::miPLIters) to use < for parallelLib send/recv

Private Attributes

- int paramsMsgLen

    length of MPI buffer for parameter input instance(s)

- int resultsMsgLen

    length of MPI buffer for results output instance(s)

14.96.1 Detailed Description

This class encapsulates scheduling operations for concurrent sub-iteration within an outer level context (e.g., meta-iteration, nested models).

In time, a Scheduler class hierarchy is envisioned, but for now, this class is not part of a hierarchy.

14.96.2 Constructor & Destructor Documentation

14.96.2.1 IteratorScheduler (ParallelLibrary & *parallel_lib*, bool *peer_assign_jobs*, int *num_servers* = 0, int *procs_per_iterator* = 0, short *scheduling* = DEFAULT_SCHEDULING)

constructor

Current constructor parameters are the input specification components, which are requests subject to override by ParallelLibrary::init_iterator_communicators().

14.96.3 Member Function Documentation

14.96.3.1 void init_iterator (ProblemDescDB & *problem_db*, Iterator & *sub_iterator*, ParLevLIter *pl_iter*) [static]

convenience function for allocation of an iterator and (parallel) initialization of its comms

This is a convenience function for encapsulating the allocation of communicators prior to running an iterator.

References ProblemDescDB::get_iterator(), ProblemDescDB::get_model(), ProblemDescDB::get_ushort(), Model::init_comms_bcast_flag(), Iterator::init_communicators(), Iterator::is_null(), Model::is_null(), Iterator::iterated_model(), Iterator::maximum_evaluation_concurrency(), Iterator::method_name(), Model::serve_init_communicators(), and Model::stop_init_communicators().

Referenced by MetaIterator::allocate_by_name(), MetaIterator::allocate_by_pointer(), Environment::construct(), ConcurrentMetaIterator::derived_init_communicators(), NestedModel::derived_init_communicators(), and IteratorScheduler::init_iterator().

14.96.3.2 void init_iterator (ProblemDescDB & *problem_db*, Iterator & *sub_iterator*, Model & *sub_model*, ParLevLIter *pl_iter*) [static]

convenience function for allocation of an iterator and (parallel) initialization of its comms

This is a convenience function for encapsulating the allocation of communicators prior to running an iterator.

References ProblemDescDB::get_iterator(), ProblemDescDB::get_ushort(), Model::init_comms_bcast_flag(), Iterator::init_communicators(), Iterator::is_null(), Iterator::iterated_model(), Iterator::maximum_evaluation_concurrency(), Iterator::method_name(), Model::serve_init_communicators(), and Model::stop_init_communicators().

14.96.3.3 void init_iterator (ProblemDescDB & *problem_db*, const String & *method_string*, Iterator & *sub_iterator*, Model & *sub_model*, ParLevLIter *pl_iter*) [static]

convenience function for lightweight allocation of an iterator and (parallel) initialization of its comms

This is a convenience function for encapsulating the allocation of communicators prior to running an iterator.

References ProblemDescDB::get_iterator(), Model::init_comms_bcast_flag(), Iterator::init_communicators(), Iterator::is_null(), Iterator::iterated_model(), Iterator::maximum_evaluation_concurrency(), Iterator::method_string(), Model::serve_init_communicators(), and Model::stop_init_communicators().

14.96.3.4 void set_iterator (Iterator & *sub_iterator*, ParLevLIter *pl_iter*) [static]

convenience function for setting comms prior to running an iterator

This is a convenience function for encapsulating the deallocation of communicators after running an iterator.

References Iterator::derived_set_communicators(), and Iterator::set_communicators().

Referenced by CollabHybridMetaIterator::derived_set_communicators(), EmbedHybridMetaIterator::derived_set_communicators(), ConcurrentMetaIterator::derived_set_communicators(), SeqHybridMetaIterator::derived_set_communicators(), NestedModel::derived_set_communicators(), and IteratorScheduler::set_iterator().

14.96.3.5 void run_iterator (Iterator & *sub_iterator*, ParLevLIter *pl_iter*) [static]

Convenience function for invoking an iterator and managing parallelism. This version omits communicator repartitioning. Function must be public due to use by MINLPNode.

This is a convenience function for encapsulating the parallel features (run/serve) of running an iterator. This function omits allocation/deallocation of communicators to provide greater efficiency in approaches that involve multiple iterator executions but only require communicator allocation/deallocation to be performed once.

References Model::finalize_mapping(), Model::initialize_mapping(), Iterator::iterated_model(), Iterator::maximum-_evaluation_concurrency(), Iterator::method_name(), Iterator::resize(), Iterator::resize_communicators(), Iterator-::run(), Model::serve_finalize_mapping(), Model::serve_init_mapping(), Model::serve_run(), Model::stop_finalize_-mapping(), Model::stop_init_mapping(), and Model::stop_servers().

Referenced by NestedModel::derived_evaluate(), Environment::execute(), IteratorScheduler::peer_static_schedule-_iterators(), IteratorScheduler::run_iterator(), and IteratorScheduler::serve_iterators().

14.96.3.6 void free_iterator (Iterator & *sub_iterator*, ParLevLIter *pl_iter*) [static]

convenience function for deallocating comms after running an iterator

This is a convenience function for encapsulating the deallocation of communicators after running an iterator.

References Iterator::derived_free_communicators(), Iterator::free_communicators(), and Iterator::method_name().

Referenced by CollabHybridMetaIterator::derived_free_communicators(), EmbedHybridMetaIterator::derived_free-_communicators(), ConcurrentMetaIterator::derived_free_communicators(), SeqHybridMetaIterator::derived_free-_communicators(), NestedModel::derived_free_communicators(), Environment::destruct(), and IteratorScheduler-::free_iterator().

14.96.3.7 IntIntPair configure (ProblemDescDB & *problem_db*, Iterator & *sub_iterator*, Model & *sub_model*)

performs sufficient initialization to define partitioning controls (min and max processors per iterator server)

This is a convenience function for computing the minimum and maximum partition size prior to concurrent iterator partitioning.

References ProblemDescDB::get_iterator(), IteratorScheduler::schedPCIter, and ParallelLevel::server_communicator-_rank().

Referenced by IteratorScheduler::configure(), ConcurrentMetaIterator::derived_init_communicators(), Nested-Model::derived_init_communicators(), MetaIterator::estimate_by_name(), and MetaIterator::estimate_by_pointer().

14.96.3.8 IntIntPair configure (ProblemDescDB & *problem_db*, const String & *method_string*, Iterator & *sub_iterator*, Model & *sub_model*)

performs sufficient initialization to define partitioning controls (min and max processors per iterator server)

This is a convenience function for computing the minimum and maximum partition size prior to concurrent iterator partitioning.

References IteratorScheduler::configure(), ProblemDescDB::get_iterator(), IteratorScheduler::schedPCIter, and ParallelLevel::server_communicator_rank().

14.96.3.9 IntIntPair configure (ProblemDescDB & *problem_db*, Iterator & *sub_iterator*)

performs sufficient initialization to define partitioning controls (min and max processors per iterator server)

This is a convenience function for computing the minimum and maximum partition size prior to concurrent iterator partitioning.

References ParallelLibrary::bcast(), Iterator::estimate_partition_bounds(), ProblemDescDB::get_db_method_-node(), ProblemDescDB::get_db_model_node(), IteratorScheduler::parallelLib, IteratorScheduler::schedPCIter, ParallelLevel::server_communicator_rank(), ParallelLevel::server_communicator_size(), ProblemDescDB::set_db-_method_node(), ProblemDescDB::set_db_model_nodes(), and MPIPackBuffer::size().

14.96.3.10 void partition (int *max_iterator_concurrency,* IntIntPair & *ppi_pr*)

convenience function for initializing iterator communicators, setting parallel configuration attributes, and managing outputs and restart.

Called from derived class constructors once maxIteratorConcurrency is defined but prior to instantiating Iterators and Models.

References ParallelLibrary::init_iterator_communicators(), IteratorScheduler::iteratorScheduling, IteratorScheduler-::numIteratorServers, ParallelLibrary::parallel_configuration_iterator(), IteratorScheduler::parallelLib, Iterator-Scheduler::procsPerIterator, ParallelLibrary::push_output_tag(), and IteratorScheduler::update().

Referenced by CollabHybridMetaIterator::derived_init_communicators(), EmbedHybridMetaIterator::derived_init-_communicators(), ConcurrentMetaIterator::derived_init_communicators(), SeqHybridMetaIterator::derived_init_-communicators(), and NestedModel::derived_init_communicators().

14.96.3.11 void schedule_iterators (MetaType & *meta_object,* Iterator & *sub_iterator*)

short convenience function for distributing control among master_dynamic_schedule_iterators(), serve_iterators(), and peer_static_schedule_iterators()

This implementation supports the scheduling of multiple jobs using a single iterator/model pair. Additional future (overloaded) implementations could involve independent iterator instances.

References IteratorScheduler::iteratorScheduling, IteratorScheduler::iteratorServerId, IteratorScheduler::lead_-rank(), IteratorScheduler::master_dynamic_schedule_iterators(), IteratorScheduler::numIteratorServers, Parallel-Library::parallel_configuration_iterator(), IteratorScheduler::parallelLib, IteratorScheduler::peer_static_schedule_-iterators(), IteratorScheduler::serve_iterators(), and IteratorScheduler::stop_iterator_servers().

Referenced by CollabHybridMetaIterator::core_run(), EmbedHybridMetaIterator::core_run(), ConcurrentMeta-Iterator::core_run(), NestedModel::derived_synchronize(), SeqHybridMetaIterator::run_sequential(), and Nested-Model::serve_run().

14.96.3.12 void master_dynamic_schedule_iterators (MetaType & *meta_object*)

executed by the scheduler master to manage a dynamic schedule of iterator jobs among slave iterator servers

This function is adapted from ApplicationInterface::master_dynamic_schedule_evaluations().

References ParallelLibrary::free(), ParallelLibrary::irecv_mi(), ParallelLibrary::isend_mi(), IteratorScheduler::miPL-Index, IteratorScheduler::numIteratorJobs, IteratorScheduler::numIteratorServers, IteratorScheduler::parallelLib, M-PIPackBuffer::reset(), MPIUnpackBuffer::resize(), IteratorScheduler::resultsMsgLen, ParallelLibrary::waitall(), and ParallelLibrary::waitsome().

Referenced by IteratorScheduler::schedule_iterators().

14.96.3.13 void serve_iterators (MetaType & *meta_object,* Iterator & *sub_iterator*)

executed on the slave iterator servers to perform iterator jobs assigned by the scheduler master

This function is similar in structure to ApplicationInterface::serve_evaluations_synch().

References ParallelLibrary::bcast_i(), IteratorScheduler::iteratorCommRank, IteratorScheduler::iteratorCommSize, IteratorScheduler::miPLIndex, ParallelLibrary::parallel_time(), IteratorScheduler::parallelLib, IteratorScheduler-::paramsMsgLen, ParallelLibrary::recv_mi(), IteratorScheduler::resultsMsgLen, IteratorScheduler::run_iterator(), and ParallelLibrary::send_mi().

Referenced by IteratorScheduler::schedule_iterators().

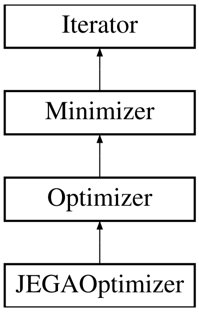
The documentation for this class was generated from the following files:

- IteratorScheduler.hpp
- IteratorScheduler.cpp

14.97 JEGAOptimizer Class Reference

A version of Dakota::Optimizer for instantiation of John Eddy's Genetic Algorithms (JEGA).

Inheritance diagram for JEGAOptimizer:



Classes

- class Driver

  A subclass of the JEGA front end driver that exposes the individual protected methods to execute the algorithm.
- class Evaluator

  An evaluator specialization that knows how to interact with Dakota.
- class EvaluatorCreator

  A specialization of the JEGA::FrontEnd::EvaluatorCreator that creates a new instance of a Evaluator.

Public Member Functions

- virtual void core_run ()

  Performs the iterations to determine the optimal set of solutions.
- virtual bool accepts_multiple_points () const

  Overridden to return true since JEGA algorithms can accept multiple initial points.
- virtual bool returns_multiple_points () const

  Overridden to return true since JEGA algorithms can return multiple final points.
- virtual void initial_points (const VariablesArray &pts)

  Overridden to assign the _initPts member variable to the passed in collection of Dakota::Variables.
- virtual const VariablesArray & initial_points () const

  Overridden to return the collection of initial points for the JEGA algorithm created and run by this JEGAOptimizer.
- JEGAOptimizer (ProblemDescDB &problem_db, Model &model)

  Constructs a JEGAOptimizer class object.
- ∼JEGAOptimizer ()

  Destructs a JEGAOptimizer.

Protected Member Functions

- void LoadDakotaResponses (const JEGA::Utilities::Design &from, Variables &vars, Response &resp) const

    Loads the JEGA-style Design class into equivalent Dakota-style Variables and Response objects.
- void ReCreateTheParameterDatabase ()

    Destroys the current parameter database and creates a new empty one.
- void LoadTheParameterDatabase ()

    Reads information out of the known Dakota::ProblemDescDB and puts it into the current parameter database.
- void LoadAlgorithmConfig (JEGA::FrontEnd::AlgorithmConfig &aConfig)

    Completely initializes the supplied algorithm configuration.
- void LoadProblemConfig (JEGA::FrontEnd::ProblemConfig &pConfig)

    Completely initializes the supplied problem configuration.
- void LoadTheDesignVariables (JEGA::FrontEnd::ProblemConfig &pConfig)

    Adds DesignVariableInfo objects into the problem configuration object.
- void LoadTheObjectiveFunctions (JEGA::FrontEnd::ProblemConfig &pConfig)

    Adds ObjectiveFunctionInfo objects into the problem configuration object.
- void LoadTheConstraints (JEGA::FrontEnd::ProblemConfig &pConfig)

    Adds ConstraintInfo objects into the problem configuration object.
- void GetBestSolutions (const JEGA::Utilities::DesignOFSortSet &from, const JEGA::Algorithms::GeneticAlgorithm &theGA, std::multimap< RealRealPair, JEGA::Utilities::Design ∗ > &designSortMap)

    Returns up to _numBest designs sorted by DAKOTA's fitness (L2 constraint violation, then utopia or objective), taking into account the algorithm type. The front of the returned map can be viewed as a single "best".
- void GetBestMOSolutions (const JEGA::Utilities::DesignOFSortSet &from, const JEGA::Algorithms::GeneticAlgorithm &theGA, std::multimap< RealRealPair, JEGA::Utilities::Design ∗ > &designSortMap)

    Retreive the best Designs from a set of solutions assuming that they are generated by a multi objective algorithm.
- void GetBestSOSolutions (const JEGA::Utilities::DesignOFSortSet &from, const JEGA::Algorithms::GeneticAlgorithm &theGA, std::multimap< RealRealPair, JEGA::Utilities::Design ∗ > &designSortMap)

    Retreive the best Designs from a set of solutions assuming that they are generated by a single objective algorithm.
- JEGA::DoubleMatrix ToDoubleMatrix (const VariablesArray &variables) const

    Converts the items in a VariablesArray into a DoubleMatrix whereby the items in the matrix are the design variables.

Private Attributes

- EvaluatorCreator ∗ _theEvalCreator

    A pointer to an EvaluatorCreator used to create the evaluator used by JEGA in Dakota (a JEGAEvaluator).
- JEGA::Utilities::ParameterDatabase ∗ _theParamDB

    A pointer to the ParameterDatabase from which all parameters are retrieved by the created algorithms.
- VariablesArray _initPts

    An array of initial points to use as an initial population.

Additional Inherited Members

14.97.1 Detailed Description

A version of Dakota::Optimizer for instantiation of John Eddy's Genetic Algorithms (JEGA).

This class encapsulates the necessary functionality for creating and properly initializing the JEGA algorithms (MOGA and SOGA).

14.97.2 Constructor & Destructor Documentation

14.97.2.1 JEGAOptimizer (ProblemDescDB & *problem_db,* Model & *model*)

Constructs a JEGAOptimizer class object.

This method does some of the initialization work for the algorithm. In particular, it initialized the JEGA core.

Parameters

problem_db	The Dakota::ProblemDescDB with information on how the algorithm controls should be set.
model	The Dakota::Model that will be used by this optimizer for problem information, etc.

References JEGAOptimizer::_theEvalCreator, ProblemDescDB::get_int(), ProblemDescDB::get_short(), Iterator::iteratedModel, JEGAOptimizer::LoadTheParameterDatabase(), Iterator::maxEvalConcurrency, Iterator::methodName, Iterator::numFinalSolutions, and Iterator::probDescDB.

14.97.3 Member Function Documentation

14.97.3.1 void LoadDakotaResponses (const JEGA::Utilities::Design & *from*, Dakota::Variables & *vars*, Dakota::Response & *resp*) const [protected]

Loads the JEGA-style Design class into equivalent Dakota-style Variables and Response objects.

This version is meant for the case where a Variables and a Response object exist and just need to be loaded.

Parameters

from	The JEGA Design class object from which to extract the variable and response information for Dakota.
vars	The Dakota::Variables object into which to load the design variable values of *from*.
resp	The Dakota::Response object into which to load the objective function and constraint values of *from*.

References Variables::continuous_variables(), Variables::discrete_int_variables(), Variables::discrete_real_variables(), Variables::discrete_string_variable(), Response::function_values(), Response::num_functions(), and Dakota::set_index_to_value().

14.97.3.2 void LoadTheParameterDatabase ( ) [protected]

Reads information out of the known Dakota::ProblemDescDB and puts it into the current parameter database.

This should be called from the JEGAOptimizer constructor since it is the only time when the problem description database is certain to be configured to supply data for this optimizer.

Referenced by JEGAOptimizer::JEGAOptimizer().

14.97.3.3 void LoadAlgorithmConfig (JEGA::FrontEnd::AlgorithmConfig & *aConfig*) [protected]

Completely initializes the supplied algorithm configuration.

This loads the supplied configuration object with appropriate data retrieved from the parameter database.

Parameters

aConfig	The algorithm configuration object to load.

14.97.3.4 void LoadProblemConfig (JEGA::FrontEnd::ProblemConfig & *pConfig*) [protected]

Completely initializes the supplied problem configuration.

This loads the fresh configuration object using the LoadTheDesignVariables, LoadTheObjectiveFunctions, and LoadTheConstraints methods.

Parameters

pConfig	The problem configuration object to load.

14.97.3.5 void LoadTheDesignVariables (JEGA::FrontEnd::ProblemConfig & *pConfig*) [protected]

Adds DesignVariableInfo objects into the problem configuration object.

This retrieves design variable information from the ParameterDatabase and creates DesignVariableInfo's from it.

Parameters

pConfig	The problem configuration object to load.

14.97.3.6 void LoadTheObjectiveFunctions (JEGA::FrontEnd::ProblemConfig & *pConfig*) [protected]

Adds ObjectiveFunctionInfo objects into the problem configuration object.

This retrieves objective function information from the ParameterDatabase and creates ObjectiveFunctionInfo's from it.

Parameters

pConfig	The problem configuration object to load.

14.97.3.7 void LoadTheConstraints (JEGA::FrontEnd::ProblemConfig & *pConfig*) [protected]

Adds ConstraintInfo objects into the problem configuration object.

This retrieves constraint function information from the ParameterDatabase and creates ConstraintInfo's from it.

Parameters

pConfig	The problem configuration object to load.

References Dakota::asstring(), and Dakota::copy_row_vector().

14.97.3.8 void GetBestSolutions (const JEGA::Utilities::DesignOFSortSet & *from,* const JEGA::Algorithms::GeneticAlgorithm & *theGA,* std::multimap< RealRealPair, JEGA::Utilities::Design ∗ > & *designSortMap*) [protected]

Returns up to _numBest designs sorted by DAKOTA's fitness (L2 constraint violation, then utopia or objective), taking into account the algorithm type. The front of the returned map can be viewed as a single "best".

Parameters

from	The full set of designs returned by the solver.
theGA	The GA used to generate this set; needed for its weights in the SO case, provided to both for consistency
designSortMap	Map of best solutions with key pair<constraintViolation, fitness>

eventually this functionality must be moved into a separate post-processing application for MO datasets.

14.97.3.9 void GetBestMOSolutions (const JEGA::Utilities::DesignOFSortSet & *from,* const JEGA::Algorithms::- GeneticAlgorithm & *theGA,* std::multimap< RealRealPair, JEGA::Utilities::Design ∗ > & *designSortMap*) [protected]

Retreive the best Designs from a set of solutions assuming that they are generated by a multi objective algorithm.

eventually this functionality must be moved into a separate post-processing application for MO datasets.

14.97.3.10 void GetBestSOSolutions (const JEGA::Utilities::DesignOFSortSet & *from*, const JEGA::Algorithms::GeneticAlgorithm & *theGA*, std::multimap< RealRealPair, JEGA::Utilities::Design * > & *designSortMap*) [protected]

Retreive the best Designs from a set of solutions assuming that they are generated by a single objective algorithm.

eventually this functionality must be moved into a separate post-processing application for MO datasets.

References Dakota::abort_handler().

14.97.3.11 JEGA::DoubleMatrix ToDoubleMatrix (const VariablesArray & *variables*) const [protected]

Converts the items in a VariablesArray into a DoubleMatrix whereby the items in the matrix are the design variables.

The matrix will not contain responses but when being used by Dakota, this doesn't matter. JEGA will attempt to re-evaluate these points but Dakota will recognize that they do not require re-evaluation and thus it will be a cheap operation.

Parameters

variables	The array of DakotaVariables objects to use as the contents of the returned matrix.

Returns

The matrix created using the supplied VariablesArray.

14.97.3.12 void core_run ( ) [virtual]

Performs the iterations to determine the optimal set of solutions.

Override of pure virtual method in Optimizer base class.

The extraction of parameter values actually occurs in this method when the JEGA::FrontEnd::Driver::ExecuteAlgorithm is called. Also the loading of the problem and algorithm configurations occurs in this method. That way, if it is called more than once and the algorithm or problem has changed, it will be accounted for.

Reimplemented from Iterator.

References JEGAOptimizer::Driver::DestroyAlgorithm(), JEGAOptimizer::Driver::ExtractAllData(), and JEGAOptimizer::Driver::PerformIterations().

14.97.3.13 bool accepts_multiple_points ( ) const [virtual]

Overridden to return true since JEGA algorithms can accept multiple initial points.

Returns

true, always.

Reimplemented from Iterator.

14.97.3.14 bool returns_multiple_points ( ) const [virtual]

Overridden to return true since JEGA algorithms can return multiple final points.

Returns

true, always.

Reimplemented from Iterator.

14.97.3.15 void initial_points (const VariablesArray & *pts*) [virtual]

Overridden to assign the _initPts member variable to the passed in collection of Dakota::Variables.

Parameters

pts	The array of initial points for the JEGA algorithm created and run by this JEGAOptimizer.

Reimplemented from Iterator.

14.97.3.16 const VariablesArray & initial_points ( ) const [virtual]

Overridden to return the collection of initial points for the JEGA algorithm created and run by this JEGAOptimizer.

Returns

The collection of initial points for the JEGA algorithm created and run by this JEGAOptimizer.

Reimplemented from Iterator.

14.97.4 Member Data Documentation

14.97.4.1 VariablesArray _initPts [private]

An array of initial points to use as an initial population.

This member is here to help support the use of JEGA algorithms in Dakota strategies. If this array is populated, then whatever initializer is specified will be ignored and the DoubleMatrix initializer will be used instead on a matrix created from the data in this array.

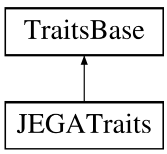
The documentation for this class was generated from the following files:

- JEGAOptimizer.hpp
- JEGAOptimizer.cpp

14.98 JEGATraits Class Reference

A version of TraitsBase specialized for John Eddy's Genetic Algorithms (JEGA).

Inheritance diagram for JEGATraits:



Public Member Functions

- JEGATraits ()

    default constructor
- virtual ∼JEGATraits ()

    destructor
- virtual bool is_derived ()

    A temporary query used in the refactor.
- bool supports_continuous_variables ()

    Return the flag indicating whether method supports continuous variables.
- bool supports_discrete_variables ()

Return the flag indicating whether method supports continuous variables.

- bool supports_linear_equality ()

  Return the flag indicating whether method supports linear equalities.

- bool supports_linear_inequality ()

  Return the flag indicating whether method supports linear inequalities.

- bool supports_nonlinear_equality ()

  Return the flag indicating whether method supports nonlinear equalities.

- bool supports_nonlinear_inequality ()

  Return the flag indicating whether method supports nonlinear inequalities.

- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()

  Return the format used for nonlinear inequality constraints.

14.98.1 Detailed Description

A version of TraitsBase specialized for John Eddy's Genetic Algorithms (JEGA).

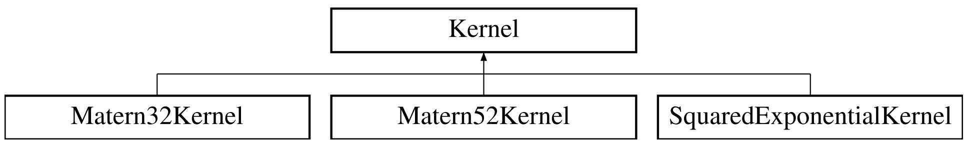
The documentation for this class was generated from the following file:

- JEGAOptimizer.hpp

14.99 Kernel Class Reference

Kernel functions for the Gaussian Process surrogate.

Inheritance diagram for Kernel:



Public Member Functions

- virtual void compute_gram (const std::vector< MatrixXd > &dists2, const VectorXd &theta_values, MatrixXd &gram)=0

  Compute a Gram matrix given a vector of squared distances and kernel hyperparameters.

- virtual void compute_gram_derivs (const MatrixXd &gram, const std::vector< MatrixXd > &dists2, const VectorXd &theta_values, std::vector< MatrixXd > &gram_derivs)=0

  Compute the derivatives of the Gram matrix with respect to the kernel hyperparameters.

- virtual MatrixXd compute_first_deriv_pred_gram (const MatrixXd &pred_gram, const std::vector< MatrixXd > &mixed_dists, const VectorXd &theta_values, const int index)=0

  Compute the first derivatve of the prediction matrix for a given component.

- virtual MatrixXd compute_second_deriv_pred_gram (const MatrixXd &pred_gram, const std::vector< Matrix-Xd > &mixed_dists, const VectorXd &theta_values, const int index_i, const int index_j)=0

  Compute the second derivatve of the prediction matrix for a pair of components.

Protected Member Functions

- void compute_Dbar (const std::vector< MatrixXd > &cw_dists2, const VectorXd &theta_values, bool take_-sqrt=true)

  Compute the "Dbar" matrices of scaled distances.

Protected Attributes

- MatrixXd **Dbar**
- MatrixXd **Dbar2**

14.99.1 Detailed Description

Kernel functions for the Gaussian Process surrogate.

14.99.2 Member Function Documentation

14.99.2.1 virtual void compute_gram (const std::vector< **MatrixXd** > & *dists2*, const **VectorXd** & *theta_values*, **MatrixXd** & *gram*) [pure virtual]

Compute a Gram matrix given a vector of squared distances and kernel hyperparameters.

Parameters

in	*dists2*	Vector of squared distance matrices.
in	*theta_values*	Vector of hyperparameters.
in,out	*gram*	Gram matrix.

Returns

Gram matrix.

Implemented in Matern52Kernel, Matern32Kernel, and SquaredExponentialKernel.

14.99.2.2 virtual void compute_gram_derivs (const **MatrixXd** & *gram*, const std::vector< **MatrixXd** > & *dists2*, const **VectorXd** & *theta_values*, std::vector< **MatrixXd** > & *gram_derivs*) [pure virtual]

Compute the derivatives of the Gram matrix with respect to the kernel hyperparameters.

Parameters

in	*gram*	Gram Matrix
in	*dists2*	Vector of squared distance matrices.
in	*theta_values*	Vector of hyperparameters.
in,out	*gram_derivs*	Vector of Gram matrix derivatives.

Returns

Derivatives of the Gram matrix w.r.t. the hyperparameters.

Implemented in Matern52Kernel, Matern32Kernel, and SquaredExponentialKernel.

14.99.2.3 virtual **MatrixXd** compute_first_deriv_pred_gram (const **MatrixXd** & *pred_gram*, const std::vector< **MatrixXd** > & *mixed_dists*, const **VectorXd** & *theta_values*, const int *index*) [pure virtual]

Compute the first derivatve of the prediction matrix for a given component.

Parameters

in	*pred_gram*	Prediction Gram matrix - Rectangular matrix of kernel evaluations between the surrogate and prediction points.
in	*mixed_dists*	Component-wise signed distances between the prediction and build points.
in	*theta_values*	Vector of hyperparameters.
in	*index*	Specifies the component of the derivative.

Returns

first_deriv_pred_gram First derivative of the prediction Gram matrix for a given component.

Implemented in Matern52Kernel, Matern32Kernel, and SquaredExponentialKernel.

14.99.2.4 virtual MatrixXd compute_second_deriv_pred_gram (const MatrixXd & *pred_gram*, const std::vector< MatrixXd > & *mixed_dists*, const VectorXd & *theta_values*, const int *index_i*, const int *index_j*) [pure virtual]

Compute the second derivatve of the prediction matrix for a pair of components.

Parameters

in	*pred_gram*	Prediction Gram matrix - Rectangular matrix of kernel evaluations between the surrogate and prediction points.
in	*mixed_dists*	Component-wise signed distances between the prediction and build points.
in	*theta_values*	Vector of hyperparameters.
in	*index_i*	Specifies the first component of the second derivative.
in	*index_j*	Specifies the second component of the second derivative.

Returns

second_deriv_pred_gram Second derivative of the prediction matrix for a pair of components.

Implemented in Matern52Kernel, Matern32Kernel, and SquaredExponentialKernel.

14.99.2.5 void compute_Dbar (const std::vector< MatrixXd > & *cw_dists2*, const VectorXd & *theta_values*, bool *take_sqrt* = true) [protected]

Compute the “Dbar” matrices of scaled distances.

Parameters

in	*cw_dists2*	Vector of component-wise squared distance matrices.
in	*theta_values*	Vector of hyperparameters.
in	*take_sqrt*	Flag for computing the square root of Dbar2.

Returns

Matrix of hyperparameter-scaled distances.

Referenced by Matern32Kernel::compute_first_deriv_pred_gram(), Matern52Kernel::compute_first_deriv_pred_gram(), SquaredExponentialKernel::compute_gram(), Matern32Kernel::compute_gram(), Matern52Kernel::compute_gram(), Matern32Kernel::compute_gram_derivs(), Matern52Kernel::compute_gram_derivs(), and Matern52Kernel::compute_second_deriv_pred_gram().

The documentation for this class was generated from the following files:

- SurrogatesGPKernels.hpp
- SurrogatesGPKernels.cpp

14.100 LabelsWriter Class Reference

Utility used in derived write_core to write labels in tabular format.

Public Member Functions

- template<typename ArrayType >
  void operator() (std::ostream &s, size_t start_index, size_t num_items, const ArrayType &array_data, StringMultiArrayConstView label_array)

14.100.1 Detailed Description

Utility used in derived write_core to write labels in tabular format.

14.100.2 Member Function Documentation

14.100.2.1 void operator() (std::ostream & *s*, size_t *start_index*, size_t *num_items*, const ArrayType & *array_data*, StringMultiArrayConstView *label_array*) [inline]

The tabular labels writer only forwards the label arrays

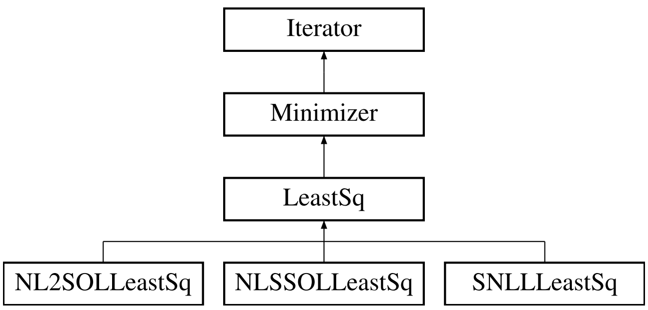
The documentation for this class was generated from the following file:

- DakotaVariables.hpp

14.101 LeastSq Class Reference

Base class for the nonlinear least squares branch of the iterator hierarchy.

Inheritance diagram for LeastSq:



Protected Member Functions

- LeastSq (std::shared_ptr< TraitsBase > traits)

  default constructor
- LeastSq (ProblemDescDB &problem_db, Model &model, std::shared_ptr< TraitsBase > traits)

  standard constructor
- LeastSq (unsigned short method_name, Model &model, std::shared_ptr< TraitsBase > traits)

  alternate "on the fly" constructor
- ∼LeastSq ()

  destructor

- void initialize_run ()
- void post_run (std::ostream &s)
- void finalize_run ()

  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)
- void get_confidence_intervals (const Variables &native_vars, const Response &iter_resp)

  Calculate confidence intervals on estimated parameters.

Protected Attributes

- size_t numLeastSqTerms

  number of least squares terms
- LeastSq ∗ prevLSqInstance

  pointer containing previous value of leastSqInstance
- bool weightFlag

  flag indicating whether weighted least squares is active
- RealVector confBoundsLower

  lower bounds for confidence intervals on calibration parameters
- RealVector confBoundsUpper

  upper bounds for confidence intervals on calibration parameters
- RealVector bestIterPriFns

  storage for iterator best primary functions (which shouldn't be stored in bestResponseArray when there are transformations)
- bool retrievedIterPriFns

  whether final primary iterator space functions have been retrieved (possibly by a derived class)

Static Protected Attributes

- static LeastSq ∗ leastSqInstance

  pointer to LeastSq instance used in static member functions

Private Member Functions

- void weight_model ()

  Wrap iteratedModel in a RecastModel that weights the residuals.
- void archive_best_results ()

  top-level archival method

Additional Inherited Members

14.101.1 Detailed Description

Base class for the nonlinear least squares branch of the iterator hierarchy.

The LeastSq class provides common data and functionality for least squares solvers (including NL2OL, NLSSOL-LeastSq, and SNLLLeastSq.

14.101.2 Constructor & Destructor Documentation

14.101.2.1 LeastSq (ProblemDescDB & *problem_db,* Model & *model,* std::shared_ptr< TraitsBase > *traits*) [protected]

standard constructor

This constructor extracts the inherited data for the least squares branch and performs sanity checking on gradient and constraint settings.

References Dakota::abort_handler(), Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, Variables::copy(), Model::current_variables(), Minimizer::data_transform_model(), Iterator::iteratedModel, Iterator::methodName, LeastSq::numLeastSqTerms, Minimizer::numTotalCalibTerms, Minimizer::optimizationFlag, Model::primary_fn_-type(), Minimizer::scale_model(), Minimizer::scaleFlag, LeastSq::weight_model(), and LeastSq::weightFlag.

14.101.3 Member Function Documentation

14.101.3.1 void initialize_run ( ) [protected], [virtual]

This function should be invoked (or reimplemented) by any derived implementations of initialize_run() (which would otherwise hide it).

Reimplemented from Iterator.

Reimplemented in SNLLLeastSq.

References LeastSq::bestIterPriFns, Minimizer::initialize_run(), Iterator::iteratedModel, LeastSq::leastSqInstance, Iterator::myModelLayers, LeastSq::prevLSqInstance, LeastSq::retrievedIterPriFns, and Model::update_from_-subordinate_model().

Referenced by SNLLLeastSq::initialize_run().

14.101.3.2 void post_run (std::ostream & *s*) [protected], [virtual]

Implements portions of post_run specific to LeastSq for scaling back to native variables and functions. This function should be invoked (or reimplemented) by any derived implementations of post_run() (which would otherwise hide it).

Reimplemented from Iterator.

References Dakota::abort_handler(), Iterator::activeSet, LeastSq::bestIterPriFns, Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, Variables::continuous_variables(), Model::continuous-_variables(), Response::copy(), Variables::copy(), Dakota::copy_data_partial(), Model::current_response(), Model-::db_lookup(), Model::evaluate(), Response::function_gradients(), Response::function_values(), Response-::function_values_view(), LeastSq::get_confidence_intervals(), Iterator::iteratedModel, Model::model_rep(), Minimizer::numContinuousVars, LeastSq::numLeastSqTerms, Minimizer::numNonlinearConstraints, Minimizer-::numUserPrimaryFns, Minimizer::original_model(), Iterator::outputLevel, Minimizer::post_run(), ActiveSet::request-_value(), ActiveSet::request_values(), ActiveSet::request_vector(), LeastSq::retrievedIterPriFns, Minimizer::scale-Flag, Minimizer::scalingModel, Minimizer::vendorNumericalGradFlag, and LeastSq::weightFlag.

14.101.3.3 void finalize_run ( ) [inline], [protected], [virtual]

utility function to perform common operations following post_run(); deallocation and resetting of instance pointers

Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's finalize_run(), typically *after* performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in SNLLLeastSq.

References Minimizer::finalize_run(), LeastSq::leastSqInstance, and LeastSq::prevLSqInstance.

Referenced by SNLLLeastSq::finalize_run().

14.101.3.4 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

Redefines default iterator results printing to include nonlinear least squares results (residual terms and constraints).

Reimplemented from Iterator.

References Iterator::activeSet, Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, LeastSq::confBoundsLower, LeastSq::confBoundsUpper, Model::continuous_variable_labels(), Minimizer::dataTransformModel, Minimizer::expData, Model::interface_id(), Iterator::iteratedModel, Model::model_rep(), ExperimentData::num_config_vars(), ExperimentData::num_experiments(), Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, Minimizer::numUserPrimaryFns, Minimizer::original_model(), Minimizer::print_best_eval_ids(), DataTransformModel::print_best_responses(), Minimizer::print_residuals(), ActiveSet::request_values(), Model::response_size(), Minimizer::scaleFlag, LeastSq::weightFlag, Variables::write(), and Dakota::write_precision.

14.101.3.5 void get_confidence_intervals (const Variables & *native_vars*, const Response & *iter_resp*) [protected]

Calculate confidence intervals on estimated parameters.

Calculate individual confidence intervals for each parameter, based on a linear approximation of the nonlinear model. native_cv are needed for transformations and final reporting. iter_resp must contain the final differenced, scaled, weighted residuals and gradients.

References LeastSq::confBoundsLower, LeastSq::confBoundsUpper, Variables::continuous_variables(), Response::copy(), Response::function_gradients_view(), Response::function_values(), Model::model_rep(), Minimizer::numContinuousVars, LeastSq::numLeastSqTerms, ScalingModel::response_modify_s2n(), Minimizer::scaleFlag, Minimizer::scalingModel, and Minimizer::vendorNumericalGradFlag.

Referenced by LeastSq::post_run().

14.101.3.6 void weight_model ( ) [private]

Wrap iteratedModel in a RecastModel that weights the residuals.

Setup Recast for weighting model. The weighting transformation doesn't resize, and makes no vars, active set or secondary mapping. All indices are one-to-one mapped (no change in counts).

References Dakota::abort_handler(), Model::assign_rep(), Iterator::iteratedModel, Iterator::myModelLayers, Iterator::outputLevel, and Model::primary_response_fn_weights().

Referenced by LeastSq::LeastSq().

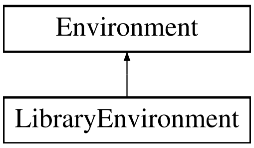
The documentation for this class was generated from the following files:

- DakotaLeastSq.hpp
- DakotaLeastSq.cpp

14.102 LibraryEnvironment Class Reference

Environment corresponding to execution as an embedded library.

Inheritance diagram for LibraryEnvironment:



Public Member Functions

- LibraryEnvironment ()

    default constructor

- LibraryEnvironment (ProgramOptions prog_opts, bool check_bcast_construct=true, DbCallbackFunctionPtr callback=NULL, void ∗callback_data=NULL)

    Primary constructor: program options typically specifies an input file or input string. Optionally specify a callback function to be invoked after parsing. Set check_bcast_construct if performing late updates and later calling done_-modifying_db().

- LibraryEnvironment (MPI_Comm dakota_mpi_comm, ProgramOptions prog_opts=ProgramOptions(), bool check_bcast_construct=true, DbCallbackFunctionPtr callback=NULL, void ∗callback_data=NULL)

    Alternate constructor accepting communicator, same options as primary.

- ∼LibraryEnvironment ()

    destructor

- void insert_nodes (Dakota::DataMethod &dme, Dakota::DataModel &dmo, Dakota::DataVariables &dv, Dakota::DataInterface &di, Dakota::DataResponses &dr)

    Insert DB nodes for a {Method,Model,Variables,Interface,Responses} set.

- void done_modifying_db ()

    Check database contents, broadcast, and construct iterators.

- bool plugin_interface (const String &model_type, const String &interf_type, const String &an_driver, Interface ∗plugin_iface)

    DEPRECATED raw pointer version: transfers memory ownership to Dakota Plug-in the passed interface into any interface matching the specified (possibly empty) model, interface, and driver strings; returns true if a plugin was performed.

- bool plugin_interface (const String &model_type, const String &interf_type, const String &an_driver, std::shared_ptr< Interface > plugin_iface)

    Plug-in the passed interface into any interface matching the specified (possibly empty) model, interface, and driver strings; returns true if a plugin was performed.

- InterfaceList filtered_interface_list (const String &interf_type, const String &an_driver)

    filter the available Interface instances based on matching interface type and analysis drivers (empty String matches any)

- ModelList filtered_model_list (const String &model_type, const String &interf_type, const String &an_driver)

    filter the available Model instances based on matching model type, interface type, and analysis drivers (empty String matches any)

Additional Inherited Members

14.102.1 Detailed Description

Environment corresponding to execution as an embedded library.

This environment corresponds to use of Dakota as a library within another application, e.g., within library_mode.cpp. It sets up the ParallelLibrary and ProblemDescDB objects without access to command line arguments.

14.102.2 Constructor & Destructor Documentation

14.102.2.1 LibraryEnvironment (ProgramOptions *prog_opts*, bool *check_bcast_construct* = `true`, DbCallbackFunctionPtr *callback* = `NULL`, void * *callback_data* = `NULL`)

Primary constructor: program options typically specifies an input file or input string. Optionally specify a callback function to be invoked after parsing. Set check_bcast_construct if performing late updates and later calling done_-modifying_db().

Construct library environment, optionally performing check/bcast of database and iterator construction

References Environment::construct(), OutputManager::output_startup_message(), Environment::outputManager, and Environment::parse().

14.102.2.2 LibraryEnvironment (MPI_Comm *dakota_mpi_comm*, ProgramOptions *prog_opts* = ProgramOptions `()`, bool *check_bcast_construct* = `true`, DbCallbackFunctionPtr *callback* = `NULL`, void * *callback_data* = `NULL`)

Alternate constructor accepting communicator, same options as primary.

Construct library environment on passed MPI Comm, optionally performing check/bcast of database and iterator construction. MPI Comm is first argument so client doesn't have to pass all args

References Environment::construct(), OutputManager::output_startup_message(), Environment::outputManager, and Environment::parse().

14.102.3 Member Function Documentation

14.102.3.1 bool plugin_interface (const String & *model_type*, const String & *interf_type*, const String & *an_driver*, Interface * *plugin_iface*)

DEPRECATED raw pointer version: transfers memory ownership to Dakota Plug-in the passed interface into any interface matching the specified (possibly empty) model, interface, and driver strings; returns true if a plugin was performed.

DEPRECATED raw pointer API; assumes memory ownership is transferred to Dakota as API historically did.

Referenced by serial_interface_plugin().

14.102.3.2 InterfaceList filtered_interface_list (const String & *interf_type*, const String & *an_driver*)

filter the available Interface instances based on matching interface type and analysis drivers (empty String matches any)

This convenience function helps clients locate and plugin to the right Interface instance for simple cases. Pass an empty string to match any instead of a specific instance

References Interface::analysis_drivers(), Dakota::contains(), Interface::interface_type(), ProblemDescDB::model_-list(), and Environment::probDescDB.

14.102.3.3 ModelList filtered_model_list (const String & *model_type*, const String & *interf_type*, const String & *an_driver*)

filter the available Model instances based on matching model type, interface type, and analysis drivers (empty String matches any)

This convenience function helps clients locate and plugin to the right Interface instance for cases where the parallel configuration is needed in constructing a parallel plugin. Pass an empty string to match any instead of a specific instance

References Interface::analysis_drivers(), Dakota::contains(), Interface::interface_type(), ProblemDescDB::model_-list(), and Environment::probDescDB.

Referenced by parallel_interface_plugin(), LibraryEnvironment::plugin_interface(), run_dakota(), and run_dakota_-mixed().

The documentation for this class was generated from the following files:

- LibraryEnvironment.hpp
- LibraryEnvironment.cpp

14.103 LightWtBaseConstructor Struct Reference

Dummy struct for overloading constructors used in on-the-fly Model instantiations.

Public Member Functions

- LightWtBaseConstructor (int=0)

    C++ structs can have constructors.

14.103.1 Detailed Description

Dummy struct for overloading constructors used in on-the-fly Model instantiations.

LightWtBaseConstructor is used to overload the constructor used for on-the-fly Model instantiations. Putting this struct here avoids circular dependencies.

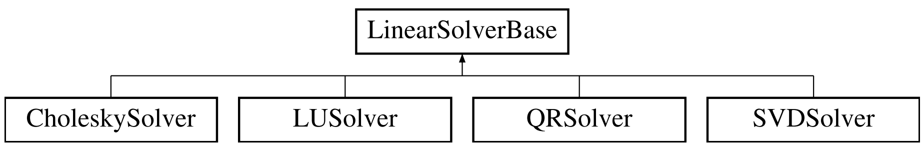
The documentation for this struct was generated from the following file:

- dakota_global_defs.hpp

14.104 LinearSolverBase Class Reference

The LinearSolverBase class serves as an API for derived solvers.

Inheritance diagram for LinearSolverBase:



Public Types

- enum SOLVER_TYPE {
CHOLESKY, **EQ_CONS_LEAST_SQ_REGRESSION**, **LASSO_REGRESSION**, **LEAST_ANGLE_REGRE-SSION**,
LU, **ORTHOG_MATCH_PURSUIT**, **QR_LEAST_SQ_REGRESSION**, **SVD_LEAST_SQ_REGRESSION** }

    How best to Doxygenate class enums? RWH.

Public Member Functions

- LinearSolverBase ()

    Constructor.

- ∼LinearSolverBase ()

  Destructor.
- virtual bool is_factorized () const

  Query to determine if the matrix of the solver has been factored.
- virtual void factorize (const MatrixXd &A)

  Perform the matrix factorization for the linear solver matrix.
- virtual void solve (const MatrixXd &A, const MatrixXd &b, MatrixXd &x)

  Find a solution to linear problem.
- virtual void solve (const MatrixXd &b, MatrixXd &x)

  Find a solution to linear problem where the LHS is already factorized.

Static Public Member Functions

- static SOLVER_TYPE solver_type (const std::string &solver_name)

  Convert solver name to enum type.

14.104.1 Detailed Description

The LinearSolverBase class serves as an API for derived solvers.

14.104.2 Member Function Documentation

14.104.2.1 SOLVER_TYPE solver_type (const std::string & *solver_name*) [static]

Convert solver name to enum type.

Parameters

in	*solver_name*	LinearSolverBase name to map

Returns

Corresponding LinearSolverBase enum

References dakota::util::type_name_bimap.

Referenced by PolynomialRegression::build().

14.104.2.2 void factorize (const MatrixXd & *A*) [virtual]

Perform the matrix factorization for the linear solver matrix.

Parameters

in	*A*	The incoming matrix to factorize.

Reimplemented in CholeskySolver, QRSolver, SVDSolver, and LUSolver.

References dakota::silence_unused_args().

14.104.2.3 void solve (const MatrixXd & *A*, const MatrixXd & *b*, MatrixXd & *x*) [virtual]

Find a solution to linear problem.

Parameters

in	*A*	The linear system left-hand-side matrix.
in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented in CholeskySolver, QRSolver, SVDSolver, and LUSolver.

References dakota::silence_unused_args().

14.104.2.4 void solve (const MatrixXd & *b*, MatrixXd & *x*) [virtual]

Find a solution to linear problem where the LHS is already factorized.

Parameters

in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented in CholeskySolver, QRSolver, SVDSolver, and LUSolver.

References dakota::silence_unused_args().

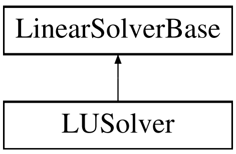
The documentation for this class was generated from the following files:

- UtilLinearSolvers.hpp
- UtilLinearSolvers.cpp

14.105 LUSolver Class Reference

The LUSolver class is used to solve linear systems with the LU decomposition.

Inheritance diagram for LUSolver:



Public Member Functions

- LUSolver ()

  Constructor.
- ∼LUSolver ()

  Destructor.
- bool is_factorized () const override

  Query to determine if the matrix of the solver has been factored.
- void factorize (const MatrixXd &A) override

  Perform the matrix factorization for the linear solver matrix.
- void solve (const MatrixXd &A, const MatrixXd &b, MatrixXd &x) override

  Find the solution to Ax = b.
- void solve (const MatrixXd &b, MatrixXd &x) override

  Find the solution to Ax = b when A is already factorized.

Private Attributes

- std::shared_ptr
  < Eigen::FullPivLU< MatrixXd > > **LU_Ptr**

Additional Inherited Members

14.105.1 Detailed Description

The LUSolver class is used to solve linear systems with the LU decomposition.

14.105.2 Member Function Documentation

14.105.2.1 void factorize (const MatrixXd & *A*) [override], [virtual]

Perform the matrix factorization for the linear solver matrix.

Parameters

in	*A*	The incoming matrix to factorize.

Reimplemented from LinearSolverBase.

Referenced by LUSolver::solve().

14.105.2.2 void solve (const MatrixXd & *A*, const MatrixXd & *b*, MatrixXd & *x*) [override], [virtual]

Find the solution to Ax = b.

Parameters

in	*A*	The linear system left-hand-side matrix.
in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented from LinearSolverBase.

References LUSolver::factorize().

14.105.2.3 void solve (const MatrixXd & *b*, MatrixXd & *x*) [override], [virtual]

Find the solution to Ax = b when A is already factorized.

Parameters

in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented from LinearSolverBase.

The documentation for this class was generated from the following files:

- UtilLinearSolvers.hpp
- UtilLinearSolvers.cpp

14.106 MatchesWC Struct Reference

Predicate that returns true when the passed path matches the wild_card with which it was configured. Currently supports $*$ and ?.

Public Member Functions

- MatchesWC (const bfs::path &wild_card)
  ctor that builds and stores the regular expression
- bool operator() (const bfs::path &dir_entry)
  return true is dir_entry matches wildCardRegEx

Public Attributes

- boost::basic_regex
  < bfs::path::value_type > wildCardRegEx
  archived RegEx; wchar-based on Windows

14.106.1 Detailed Description

Predicate that returns true when the passed path matches the wild_card with which it was configured. Currently supports ∗ and ?.

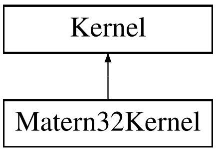
The documentation for this struct was generated from the following file:

- WorkdirHelper.hpp

14.107 Matern32Kernel Class Reference

Stationary kernel with C^1 smooth realizations.

Inheritance diagram for Matern32Kernel:



Public Member Functions

- void compute_gram (const std::vector< MatrixXd > &dists2, const VectorXd &theta_values, MatrixXd &gram) override
  Compute a Gram matrix given a vector of squared distances and kernel hyperparameters.
- void compute_gram_derivs (const MatrixXd &gram, const std::vector< MatrixXd > &dists2, const VectorXd &theta_values, std::vector< MatrixXd > &gram_derivs) override
  Compute the derivatives of the Gram matrix with respect to the kernel hyperparameters.
- MatrixXd compute_first_deriv_pred_gram (const MatrixXd &pred_gram, const std::vector< MatrixXd > &mixed_dists, const VectorXd &theta_values, const int index) override
  Compute the first derivatve of the prediction matrix for a given component.
- MatrixXd compute_second_deriv_pred_gram (const MatrixXd &pred_gram, const std::vector< MatrixXd > &mixed_dists, const VectorXd &theta_values, const int index_i, const int index_j) override
  Compute the second derivatve of the prediction matrix for a pair of components.

Private Attributes

- const double **sqrt3** = sqrt(3.)

Additional Inherited Members

14.107.1 Detailed Description

Stationary kernel with C^1 smooth realizations.

14.107.2 Member Function Documentation

14.107.2.1 void compute_gram (const std::vector< MatrixXd > & *dists2*, const VectorXd & *theta_values*, MatrixXd & *gram*) [override], [virtual]

Compute a Gram matrix given a vector of squared distances and kernel hyperparameters.

Parameters

in	*dists2*	Vector of squared distance matrices.
in	*theta_values*	Vector of hyperparameters.
in,out	*gram*	Gram matrix.

Returns

Gram matrix.

Implements Kernel.

References Kernel::compute_Dbar().

14.107.2.2 void compute_gram_derivs (const MatrixXd & *gram*, const std::vector< MatrixXd > & *dists2*, const VectorXd & *theta_values*, std::vector< MatrixXd > & *gram_derivs*) [override], [virtual]

Compute the derivatives of the Gram matrix with respect to the kernel hyperparameters.

Parameters

in	*gram*	Gram Matrix
in	*dists2*	Vector of squared distance matrices.
in	*theta_values*	Vector of hyperparameters.
in,out	*gram_derivs*	Vector of Gram matrix derivatives.

Returns

Derivatives of the Gram matrix w.r.t. the hyperparameters.

Implements Kernel.

References Kernel::compute_Dbar().

14.107.2.3 MatrixXd compute_first_deriv_pred_gram (const MatrixXd & *pred_gram*, const std::vector< MatrixXd > & *mixed_dists*, const VectorXd & *theta_values*, const int *index*) [override], [virtual]

Compute the first derivatve of the prediction matrix for a given component.

Parameters

in	*pred_gram*	Prediction Gram matrix - Rectangular matrix of kernel evaluations between the surrogate and prediction points.
in	*mixed_dists*	Component-wise signed distances between the prediction and build points.
in	*theta_values*	Vector of hyperparameters.
in	*index*	Specifies the component of the derivative.

Returns

first_deriv_pred_gram First derivative of the prediction Gram matrix for a given component.

Implements Kernel.

References dakota::surrogates::compute_cw_dists_squared(), Kernel::compute_Dbar(), and dakota::silence_-unused_args().

14.107.2.4 MatrixXd compute_second_deriv_pred_gram (const MatrixXd & *pred_gram*, const std::vector< MatrixXd > & *mixed_dists*, const VectorXd & *theta_values*, const int *index_i*, const int *index_j*) [override], [virtual]

Compute the second derivatve of the prediction matrix for a pair of components.

Parameters

in	*pred_gram*	Prediction Gram matrix - Rectangular matrix of kernel evaluations between the surrogate and prediction points.
in	*mixed_dists*	Component-wise signed distances between the prediction and build points.
in	*theta_values*	Vector of hyperparameters.
in	*index_i*	Specifies the first component of the second derivative.
in	*index_j*	Specifies the second component of the second derivative.

Returns

second_deriv_pred_gram Second derivative of the prediction matrix for a pair of components.

Implements Kernel.

References dakota::silence_unused_args().

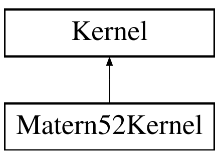
The documentation for this class was generated from the following files:

- SurrogatesGPKernels.hpp
- SurrogatesGPKernels.cpp

14.108 Matern52Kernel Class Reference

Stationary kernel with C^2 smooth realizations.

Inheritance diagram for Matern52Kernel:



Public Member Functions

- void compute_gram (const std::vector< MatrixXd > &dists2, const VectorXd &theta_values, MatrixXd &gram) override

    Compute a Gram matrix given a vector of squared distances and kernel hyperparameters.
- void compute_gram_derivs (const MatrixXd &gram, const std::vector< MatrixXd > &dists2, const VectorXd &theta_values, std::vector< MatrixXd > &gram_derivs) override

    Compute the derivatives of the Gram matrix with respect to the kernel hyperparameters.
- MatrixXd compute_first_deriv_pred_gram (const MatrixXd &pred_gram, const std::vector< MatrixXd > &mixed_dists, const VectorXd &theta_values, const int index) override

    Compute the first derivatve of the prediction matrix for a given component.
- MatrixXd compute_second_deriv_pred_gram (const MatrixXd &pred_gram, const std::vector< MatrixXd > &mixed_dists, const VectorXd &theta_values, const int index_i, const int index_j) override

    Compute the second derivatve of the prediction matrix for a pair of components.

Private Attributes

- const double **sqrt5** = sqrt(5.)

Additional Inherited Members

14.108.1 Detailed Description

Stationary kernel with C^2 smooth realizations.

14.108.2 Member Function Documentation

14.108.2.1 void compute_gram (const std::vector< MatrixXd > & *dists2*, const VectorXd & *theta_values*, MatrixXd & *gram*) [override], [virtual]

Compute a Gram matrix given a vector of squared distances and kernel hyperparameters.

Parameters

in	*dists2*	Vector of squared distance matrices.
in	*theta_values*	Vector of hyperparameters.
in,out	*gram*	Gram matrix.

Returns

Gram matrix.

Implements Kernel.

References Kernel::compute_Dbar().

14.108.2.2 void compute_gram_derivs (const MatrixXd & *gram*, const std::vector< MatrixXd > & *dists2*, const VectorXd & *theta_values*, std::vector< MatrixXd > & *gram_derivs*) [override], [virtual]

Compute the derivatives of the Gram matrix with respect to the kernel hyperparameters.

Parameters

in	*gram*	Gram Matrix
in	*dists2*	Vector of squared distance matrices.
in	*theta_values*	Vector of hyperparameters.
in,out	*gram_derivs*	Vector of Gram matrix derivatives.

Returns

Derivatives of the Gram matrix w.r.t. the hyperparameters.

Implements Kernel.

References Kernel::compute_Dbar().

14.108.2.3 MatrixXd compute_first_deriv_pred_gram (const MatrixXd & *pred_gram*, const std::vector< MatrixXd > & *mixed_dists*, const VectorXd & *theta_values*, const int *index*) [override], [virtual]

Compute the first derivatve of the prediction matrix for a given component.

Parameters

in	*pred_gram*	Prediction Gram matrix - Rectangular matrix of kernel evaluations between the surrogate and prediction points.
in	*mixed_dists*	Component-wise signed distances between the prediction and build points.
in	*theta_values*	Vector of hyperparameters.
in	*index*	Specifies the component of the derivative.

Returns

first_deriv_pred_gram First derivative of the prediction Gram matrix for a given component.

Implements Kernel.

References dakota::surrogates::compute_cw_dists_squared(), Kernel::compute_Dbar(), and dakota::silence_-unused_args().

14.108.2.4 MatrixXd compute_second_deriv_pred_gram (const MatrixXd & *pred_gram*, const std::vector< MatrixXd > & *mixed_dists*, const VectorXd & *theta_values*, const int *index_i*, const int *index_j*) [override], [virtual]

Compute the second derivatve of the prediction matrix for a pair of components.

Parameters

in	*pred_gram*	Prediction Gram matrix - Rectangular matrix of kernel evaluations between the surrogate and prediction points.
in	*mixed_dists*	Component-wise signed distances between the prediction and build points.
in	*theta_values*	Vector of hyperparameters.
in	*index_i*	Specifies the first component of the second derivative.
in	*index_j*	Specifies the second component of the second derivative.

Returns

second_deriv_pred_gram Second derivative of the prediction matrix for a pair of components.

Implements Kernel.

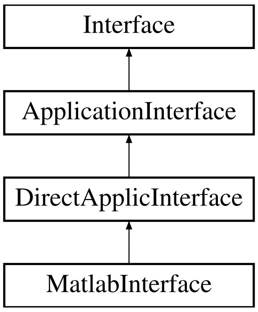
References dakota::surrogates::compute_cw_dists_squared(), Kernel::compute_Dbar(), and dakota::silence_-unused_args().

The documentation for this class was generated from the following files:

- SurrogatesGPKernels.hpp
- SurrogatesGPKernels.cpp

14.109 MatlabInterface Class Reference

Inheritance diagram for MatlabInterface:



Public Member Functions

- MatlabInterface (const ProblemDescDB &problem_db)

  Constructor: start Matlab engine.
- ∼MatlabInterface ()

  Destructor: close Matlab engine.

Protected Member Functions

- virtual int derived_map_ac (const String &ac_name)

  execute an analysis code portion of a direct evaluation invocation
- int matlab_engine_run (const Dakota::String &ac_name)

  Helper function supporting derived_map_ac. Sends data to Matlab, executes analysis, collects return data.
- int matlab_field_prep (mxArray ∗dakota_matlab, const char ∗field_name)

  check that the dakota_matlab strucutre has the specified field_name and add if necessary; free structure memory in preparation for new alloc

Protected Attributes

- engine ∗ matlabEngine

  pointer to the MATLAB engine used for direct evaluations

14.109.1 Detailed Description

Specialization of DirectApplicInterface to link to Matlab analysis drivers. Includes convenience functions to map data to/from Matlab

14.109.2 Member Function Documentation

14.109.2.1 int derived_map_ac (const String & *ac_name*) [protected], [virtual]

execute an analysis code portion of a direct evaluation invocation

Matlab specialization of dervied analysis components.

References ApplicationInterface::analysisServerId, and MatlabInterface::matlab_engine_run().

14.109.2.2 int matlab_engine_run (const Dakota::String & *ac_name*) [protected]

Helper function supporting derived_map_ac. Sends data to Matlab, executes analysis, collects return data.

Direct interface to Matlab through Mathworks external API. m-file executed is specified through analysis_drivers, extra strings through analysis_components. (Original BMA 11/28/2005)

Special thanks to Lee Peterson for substantial enhancements 12/15/2007: Added output buffer for the MATLAB command response and error messages Made the Dakota variable persistent in the MATLAB engine workspace Added robustness to the user deleting required Dakota fields

References Dakota::abort_handler(), Interface::analysisComponents, DirectApplicInterface::analysisDriverIndex, Interface::currEvalId, DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, Dakota::FIELD_NAMES, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, Interface::fnLabels, DirectApplicInterface::fnVals, DirectApplicInterface::gradFlag, DirectApplicInterface::hessFlag, MatlabInterface::matlab_field_prep(), MatlabInterface::matlabEngine, DirectApplicInterface::numACV, DirectApplicInterface::numADIV, DirectApplicInterface::numADRV, Dakota::NUMBER_OF_FIELDS, DirectApplicInterface::numDerivVars, DirectApplicInterface::numFns, DirectApplicInterface::numVars, Interface::outputLevel, DirectApplicInterface::xC, DirectApplicInterface::xCLabels, DirectApplicInterface::xDI, DirectApplicInterface::xDILabels, DirectApplicInterface::xDR, and DirectApplicInterface::xDRLabels.

Referenced by MatlabInterface::derived_map_ac().

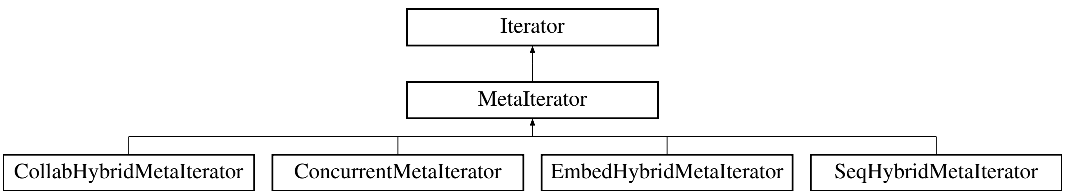
The documentation for this class was generated from the following files:

- MatlabInterface.hpp
- MatlabInterface.cpp

14.110 MetaIterator Class Reference

Base class for meta-iterators.

Inheritance diagram for MetaIterator:



Public Member Functions

- bool resize ()
  reinitializes iterator based on new variable size

Protected Member Functions

- MetaIterator (ProblemDescDB &problem_db)
  standard constructor
- MetaIterator (ProblemDescDB &problem_db, Model &model)
  alternate constructor

- ∼MetaIterator ()

  destructor
- void post_run (std::ostream &s)

  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- void check_model (const String &method_ptr, const String &model_ptr)

  check that a model identified by pointer has the same id as the iteratedModel passed through the ctor chain
- void allocate_by_pointer (const String &method_ptr, Iterator &the_iterator, Model &the_model)

  initialize the_iterator and the_model based on method_ptr
- void allocate_by_name (const String &method_string, const String &model_ptr, Iterator &the_iterator, Model &the_model)

  initialize the_iterator based on method_string
- std::pair< int, int > estimate_by_pointer (const String &method_ptr, Iterator &the_iterator, Model &the_-model)

  estimate minimum and maximum processors per iterator needed for init_iterator_parallelism(); instantiates the_-iterator and the_model as needed, but on minimal processor ranks (is later augmented by allocate_by_pointer())
- std::pair< int, int > estimate_by_name (const String &method_string, const String &model_ptr, Iterator &the-_iterator, Model &the_model)

  estimate minimum and maximum processors per iterator needed for init_iterator_parallelism(); instantiates the_-iterator and the_model as needed, but on minimal processor ranks (is later augmented by allocate_by_name())

Protected Attributes

- IteratorScheduler iterSched

  scheduler for concurrent execution of Iterators
- int maxIteratorConcurrency

  maximum number of concurrent sub-iterator executions

Additional Inherited Members

14.110.1 Detailed Description

Base class for meta-iterators.

This base class shares code for concurrent and hybrid meta-iterators, where the former supports multi-start and Pareto set iteration and the latter supports sequential, embedded, and collaborative hybrids.

14.110.2 Member Function Documentation

14.110.2.1 void post_run (std::ostream & *s*) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Iterator.

References MetaIterator::iterSched, IteratorScheduler::lead_rank(), and Iterator::print_results().

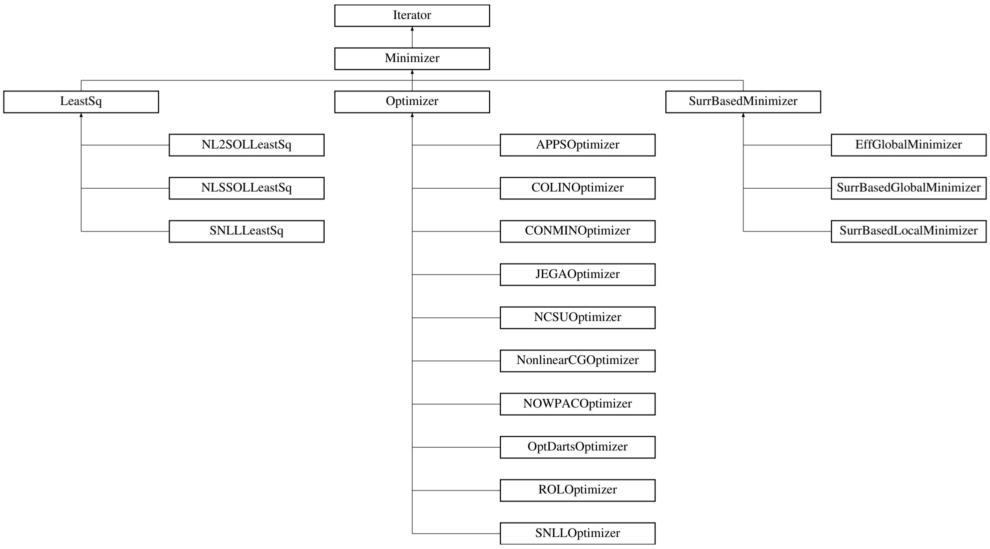
The documentation for this class was generated from the following files:

- MetaIterator.hpp
- MetaIterator.cpp

14.111 Minimizer Class Reference

Base class for the optimizer and least squares branches of the iterator hierarchy.

Inheritance diagram for Minimizer:



Public Member Functions

- void constraint_tolerance (Real constr_tol)

    set the method constraint tolerance (constraintTol)
- Real constraint_tolerance () const

    return the method constraint tolerance (constraintTol)
- std::shared_ptr< TPLDataTransfer > **get_data_transfer_helper** () const
- bool resize ()

    reinitializes iterator based on new variable size

Static Public Member Functions

- static Real sum_squared_residuals (size_t num_pri_fns, const RealVector &residuals, const RealVector &weights)

    return weighted sum of squared residuals
- static void print_residuals (size_t num_terms, const RealVector &best_terms, const RealVector &weights, size_t num_best, size_t best_index, std::ostream &s)

    print num_terms residuals and misfit for final results
- static void print_model_resp (size_t num_pri_fns, const RealVector &best_fns, size_t num_best, size_t best-_index, std::ostream &s)

    print the original user model resp in the case of data transformations
- static void print_best_eval_ids (const String &interface_id, const Variables &best_vars, const ActiveSet &active_set, std::ostream &s)

    print best evaluation matching vars and set, or partial matches with matching variables only.

Protected Member Functions

- Minimizer (std::shared_ptr< TraitsBase > traits=std::shared_ptr< TraitsBase >(new TraitsBase()))

    default constructor

- Minimizer (ProblemDescDB &problem_db, Model &model, std::shared_ptr< TraitsBase > traits=std::shared-_ptr< TraitsBase >(new TraitsBase()))

  standard constructor
- Minimizer (unsigned short method_name, Model &model, std::shared_ptr< TraitsBase > traits=std::shared-_ptr< TraitsBase >(new TraitsBase()))

  alternate constructor for "on the fly" instantiations
- Minimizer (unsigned short method_name, size_t num_lin_ineq, size_t num_lin_eq, size_t num_nln_ineq, size_t num_nln_eq, std::shared_ptr< TraitsBase > traits=std::shared_ptr< TraitsBase >(new TraitsBase()))

  alternate constructor for "on the fly" instantiations
- Minimizer (Model &model, size_t max_iter, size_t max_eval, Real conv_tol, std::shared_ptr< TraitsBase > traits=std::shared_ptr< TraitsBase >(new TraitsBase()))

  alternate constructor for "on the fly" instantiations
- ∼Minimizer ()

  destructor
- void update_from_model (const Model &model)

  set inherited data attributes based on extractions from incoming model
- void initialize_run ()

  utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
- void post_run (std::ostream &s)

  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- void finalize_run ()

  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
- const Model & algorithm_space_model () const
- Model original_model (unsigned short recasts_left=0) const

  Return a shallow copy of the original model this Iterator was originally passed, optionally leaving recasts_left on top of it.
- void data_transform_model ()

  Wrap iteratedModel in a RecastModel that subtracts provided observed data from the primary response functions (variables and secondary responses are unchanged)
- void scale_model ()

  Wrap iteratedModel in a RecastModel that performs variable and/or response scaling.
- Real objective (const RealVector &fn_vals, const BoolDeque &max_sense, const RealVector &primary_wts) const

  compute a composite objective value from one or more primary functions
- Real objective (const RealVector &fn_vals, size_t num_fns, const BoolDeque &max_sense, const RealVector &primary_wts) const

  compute a composite objective with specified number of source primary functions, instead of userPrimaryFns
- void objective_gradient (const RealVector &fn_vals, const RealMatrix &fn_grads, const BoolDeque &max_-sense, const RealVector &primary_wts, RealVector &obj_grad) const

  compute the gradient of the composite objective function
- void objective_gradient (const RealVector &fn_vals, size_t num_fns, const RealMatrix &fn_grads, const Bool-Deque &max_sense, const RealVector &primary_wts, RealVector &obj_grad) const

  compute the gradient of the composite objective function
- void objective_hessian (const RealVector &fn_vals, const RealMatrix &fn_grads, const RealSymMatrixArray &fn_hessians, const BoolDeque &max_sense, const RealVector &primary_wts, RealSymMatrix &obj_hess) const

  compute the Hessian of the composite objective function
- void objective_hessian (const RealVector &fn_vals, size_t num_fns, const RealMatrix &fn_grads, const Real-SymMatrixArray &fn_hessians, const BoolDeque &max_sense, const RealVector &primary_wts, RealSym-Matrix &obj_hess) const

  compute the Hessian of the composite objective function

- virtual void archive_best_results ()

    top-level archival method
- void archive_best_variables (const bool active_only=false) const

    archive best variables for the index'th final solution
- void archive_best_objective_functions () const

    archive the index'th set of objective functions
- void archive_best_constraints () const

    archive the index'th set of constraints
- void archive_best_residuals () const

    Archive residuals when calibration terms are used.
- void resize_best_vars_array (size_t newsize)

    Safely resize the best variables array to newsize taking into account the envelope-letter design pattern and any recasting.
- void resize_best_resp_array (size_t newsize)

    Safely resize the best response array to newsize taking into account the envelope-letter design pattern and any recasting.
- bool local_recast_retrieve (const Variables &vars, Response &response) const

    infers MOO/NLS solution from the solution of a single-objective optimizer and returns true if lookup succeeds

Protected Attributes

- size_t numFunctions

    number of response functions
- size_t numContinuousVars

    number of active continuous vars
- size_t numDiscreteIntVars

    number of active discrete integer vars
- size_t numDiscreteStringVars

    number of active discrete string vars
- size_t numDiscreteRealVars

    number of active discrete real vars
- Real constraintTol

    optimizer/least squares constraint tolerance
- Real bigRealBoundSize

    cutoff value for inequality constraint and continuous variable bounds
- int bigIntBoundSize

    cutoff value for discrete variable bounds
- size_t numNonlinearIneqConstraints

    number of nonlinear inequality constraints
- size_t numNonlinearEqConstraints

    number of nonlinear equality constraints
- size_t numLinearIneqConstraints

    number of linear inequality constraints
- size_t numLinearEqConstraints

    number of linear equality constraints
- size_t numNonlinearConstraints

    total number of nonlinear constraints
- size_t numLinearConstraints

    total number of linear constraints
- size_t numConstraints

    total number of linear and nonlinear constraints

- bool optimizationFlag

    flag for use where optimization and NLS must be distinguished
- size_t numUserPrimaryFns

    number of objective functions or least squares terms in the inbound model; always initialize at Minimizer, even if overridden later
- size_t numIterPrimaryFns

    number of objective functions or least squares terms in iterator's view, after transformations; always initialize at Minimizer, even if overridden later
- bool boundConstraintFlag

    convenience flag for denoting the presence of user-specified bound constraints. Used for method selection and error checking.
- bool speculativeFlag

    flag for speculative gradient evaluations
- bool calibrationDataFlag

    flag indicating whether user-supplied calibration data is active
- ExperimentData expData

    Container for experimental data to which to calibrate model using least squares or other formulations which minimize SSE.
- size_t numExperiments

    number of experiments
- size_t numTotalCalibTerms

    number of total calibration terms (sum over experiments of number of experimental data per experiment, including field data)
- Model dataTransformModel

    Shallow copy of the data transformation model, when present (cached in case further wrapped by other transformations)
- bool scaleFlag

    whether Iterator-level scaling is active
- Model scalingModel

    Shallow copy of the scaling transformation model, when present (cached in case further wrapped by other transformations)
- Minimizer * prevMinInstance

    pointer containing previous value of minimizerInstance
- bool vendorNumericalGradFlag

    convenience flag for gradient_type == numerical && method_source == vendor
- std::shared_ptr< TPLDataTransfer > dataTransferHandler

    Emerging helper class for handling data transfers to/from Dakota and the underlying TPL.

Static Protected Attributes

- static Minimizer * minimizerInstance

    pointer to Minimizer used in static member functions

Friends

- class SOLBase

    the SOLBase class is not derived the iterator hierarchy but still needs access to iterator hierarchy data (to avoid attribute replication)
- class SNLLBase

    the SNLLBase class is not derived the iterator hierarchy but still needs access to iterator hierarchy data (to avoid attribute replication)

Additional Inherited Members

14.111.1 Detailed Description

Base class for the optimizer and least squares branches of the iterator hierarchy.

The Minimizer class provides common data and functionality for Optimizer and LeastSq.

14.111.2 Constructor & Destructor Documentation

14.111.2.1 Minimizer (ProblemDescDB & *problem_db*, Model & *model*, std::shared_ptr< TraitsBase > *traits* = std::shared_ptr<TraitsBase>(new TraitsBase())) [protected]

standard constructor

This constructor extracts inherited data for the optimizer and least squares branches and performs sanity checking on constraint settings.

References Iterator::iteratedModel, Iterator::maxFunctionEvals, Iterator::maxIterations, Iterator::methodName, Iterator::numFinalSolutions, Dakota::SZ_MAX, and Minimizer::update_from_model().

14.111.3 Member Function Documentation

14.111.3.1 void print_best_eval_ids (const String & *search_interface_id*, const Variables & *search_vars*, const ActiveSet & *search_set*, std::ostream & *s*) [static]

print best evaluation matching vars and set, or partial matches with matching variables only.

Lookup evaluation id where best occurred. This cannot be catalogued directly because the optimizers track the best iterate internally and return the best results after iteration completion. Therfore, perform a search in data_pairs to extract the evalId for the best fn eval.

References Dakota::data_pairs, and Dakota::lookup_by_val().

Referenced by LeastSq::print_results(), SurrBasedMinimizer::print_results(), and Optimizer::print_results().

14.111.3.2 void initialize_run ( ) [protected], [virtual]

utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers

Perform initialization phases of run sequence, like allocating memory and setting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's initialize_run(), typically *before* performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in Optimizer, SNLLOptimizer, SNLLLeastSq, and ROLOptimizer.

References Model::all_continuous_variables(), Model::all_discrete_int_variables(), Model::all_discrete_real_-variables(), Iterator::bestVariablesArray, Model::initialize_mapping(), Model::is_null(), Iterator::iteratedModel, Iterator::methodPCIter, Minimizer::minimizerInstance, Iterator::myModelLayers, Minimizer::prevMinInstance, Minimizer::resize(), Model::set_evaluation_reference(), Iterator::subIteratorFlag, Model::subordinate_model(), and Iterator::summaryOutputFlag.

Referenced by LeastSq::initialize_run(), and Optimizer::initialize_run().

14.111.3.3 void post_run (std::ostream & *s*) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in Optimizer, SNLLOptimizer, EffGlobalMinimizer, and SurrBasedLocalMinimizer.

References Minimizer::archive_best_results(), Model::is_null(), Iterator::iteratedModel, Model::print_evaluation_-summary(), Iterator::print_results(), and Iterator::summaryOutputFlag.

Referenced by LeastSq::post_run(), SurrBasedLocalMinimizer::post_run(), EffGlobalMinimizer::post_run(), and Optimizer::post_run().

14.111.3.4 void finalize_run ( ) [protected], [virtual]

utility function to perform common operations following post_run(); deallocation and resetting of instance pointers

Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's finalize_run(), typically *after* performing its own implementation steps.

Reimplemented from Iterator.

Reimplemented in Optimizer, SNLLOptimizer, and SNLLLeastSq.

References Model::finalize_mapping(), Model::is_null(), Iterator::iteratedModel, Minimizer::minimizerInstance, Minimizer::prevMinInstance, and Minimizer::resize().

Referenced by LeastSq::finalize_run(), and Optimizer::finalize_run().

14.111.3.5 const Model & algorithm_space_model ( ) const [inline], [protected], [virtual]

default definition that gets redefined in selected derived Minimizers

Reimplemented from Iterator.

Reimplemented in EffGlobalMinimizer.

References Iterator::iteratedModel.

14.111.3.6 void data_transform_model ( ) [protected]

Wrap iteratedModel in a RecastModel that subtracts provided observed data from the primary response functions (variables and secondary responses are unchanged)

Reads observation data to compute least squares residuals and expands residuals for multiple experiments.

References Dakota::abort_handler(), Iterator::activeSet, Iterator::assign_rep(), Model::current_variables(), Minimizer::dataTransformModel, Minimizer::expData, ProblemDescDB::get_sizet(), Iterator::iteratedModel, ExperimentData::load_data(), Iterator::myModelLayers, ExperimentData::num_config_vars(), Model::num_primary-_fns(), Minimizer::numExperiments, Minimizer::numFunctions, Minimizer::numIterPrimaryFns, Minimizer::num-NonlinearConstraints, Minimizer::numTotalCalibTerms, Iterator::outputLevel, Iterator::probDescDB, ActiveSet-::request_vector(), and Model::response_size().

Referenced by LeastSq::LeastSq(), and Optimizer::Optimizer().

14.111.3.7 void scale_model ( ) [protected]

Wrap iteratedModel in a RecastModel that performs variable and/or response scaling.

Wrap the iteratedModel in a scaling transformation, such that iteratedModel now contains a scaling recast model. Potentially affects variables, primary, and secondary responses

References Model::assign_rep(), Iterator::iteratedModel, Iterator::myModelLayers, and Minimizer::scalingModel.

Referenced by LeastSq::LeastSq(), and Optimizer::Optimizer().

14.111.3.8 Real objective (const RealVector & *fn_vals,* const BoolDeque & *max_sense,* const RealVector & *primary_wts*) const [protected]

compute a composite objective value from one or more primary functions

The composite objective computation sums up the contributions from one of more primary functions using the primary response fn weights.

References Minimizer::numUserPrimaryFns.

Referenced by SurrBasedLocalMinimizer::approx_subprob_objective_eval(), SurrBasedMinimizer::augmented_lagrangian_merit(), EffGlobalMinimizer::compute_expected_improvement(), EffGlobalMinimizer::compute_lower_confidence_bound(), EffGlobalMinimizer::compute_probability_improvement(), SurrBasedLocalMinimizer::compute_trust_region_ratio(), SurrBasedMinimizer::initialize_filter(), SurrBasedMinimizer::lagrangian_merit(), Optimizer::objective_reduction(), SurrBasedMinimizer::penalty_merit(), COLINOptimizer::post_run(), SurrBasedMinimizer::update_filter(), and SurrBasedLocalMinimizer::update_penalty().

14.111.3.9 Real objective (const RealVector & *fn_vals,* size_t *num_fns,* const BoolDeque & *max_sense,* const RealVector & *primary_wts*) const [protected]

compute a composite objective with specified number of source primary functions, instead of userPrimaryFns

This "composite" objective is a more general case of the previous objective(), but doesn't presume a reduction map from user to iterated space. Used to apply weights and sense in COLIN results sorting. Leaving as a duplicate implementation pending resolution of COLIN lookups.

References Minimizer::optimizationFlag.

14.111.3.10 void objective_gradient (const RealVector & *fn_vals,* size_t *num_fns,* const RealMatrix & *fn_grads,* const BoolDeque & *max_sense,* const RealVector & *primary_wts,* RealVector & *obj_grad*) const [protected]

compute the gradient of the composite objective function

The composite objective gradient computation combines the contributions from one of more primary function gradients, including the effect of any primary function weights. In the case of a linear mapping (MOO), only the primary function gradients are required, but in the case of a nonlinear mapping (NLS), primary function values are also needed. Within RecastModel::set_mapping(), the active set requests are automatically augmented to make values available when needed, based on nonlinearRespMapping settings.

References Minimizer::numContinuousVars, and Minimizer::optimizationFlag.

14.111.3.11 void objective_hessian (const RealVector & *fn_vals,* size_t *num_fns,* const RealMatrix & *fn_grads,* const RealSymMatrixArray & *fn_hessians,* const BoolDeque & *max_sense,* const RealVector & *primary_wts,* RealSymMatrix & *obj_hess*) const [protected]

compute the Hessian of the composite objective function

The composite objective Hessian computation combines the contributions from one of more primary function Hessians, including the effect of any primary function weights. In the case of a linear mapping (MOO), only the primary function Hessians are required, but in the case of a nonlinear mapping (NLS), primary function values and gradients are also needed in general (gradients only in the case of a Gauss-Newton approximation). Within the default RecastModel::set_mapping(), the active set requests are automatically augmented to make values and gradients available when needed, based on nonlinearRespMapping settings.

References Dakota::abort_handler(), Minimizer::numContinuousVars, and Minimizer::optimizationFlag.

14.111.3.12 void resize_best_vars_array (size_t *newsize*) [protected]

Safely resize the best variables array to newsize taking into account the envelope-letter design pattern and any recasting.

Uses data from the innermost model, should any Minimizer recasts be active. Called by multipoint return solvers. Do not directly call resize on the bestVariablesArray object unless you intend to share the internal content (letter) with other objects after assignment.

References Iterator::bestVariablesArray, Variables::copy(), Model::current_variables(), and Minimizer::original_-model().

Referenced by COLINOptimizer::post_run().

14.111.3.13 void resize_best_resp_array (size_t *newsize*) [protected]

Safely resize the best response array to newsize taking into account the envelope-letter design pattern and any recasting.

Uses data from the innermost model, should any Minimizer recasts be active. Called by multipoint return solvers. Do not directly call resize on the bestResponseArray object unless you intend to share the internal content (letter) with other objects after assignment.

References Iterator::bestResponseArray, Response::copy(), Model::current_response(), and Minimizer::original_-model().

Referenced by COLINOptimizer::post_run().

14.111.3.14 bool local_recast_retrieve (const Variables & *vars,* Response & *response*) const [protected]

infers MOO/NLS solution from the solution of a single-objective optimizer and returns true if lookup succeeds

Retrieve a MOO/NLS response based on the data returned by a single objective optimizer by performing a data_-pairs search. This may get called even for a single user-specified function, since we may be recasting a single NLS residual into a squared objective. Always returns best data in the space of the original inbound Model.

References Response::active_set(), Dakota::data_pairs, Model::interface_id(), Iterator::iteratedModel, Dakota-::lookup_by_val(), and Response::update().

Referenced by Minimizer::archive_best_results(), and Optimizer::post_run().

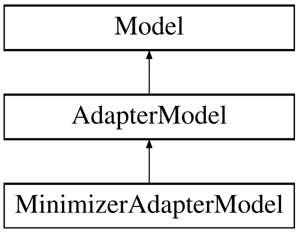
The documentation for this class was generated from the following files:

- DakotaMinimizer.hpp
- DakotaMinimizer.cpp

14.112 MinimizerAdapterModel Class Reference

Derived model class which wraps call-back functions for solving minimization sub-problems.

Inheritance diagram for MinimizerAdapterModel:



Public Member Functions

- MinimizerAdapterModel (const RealVector &cv_initial_pt, const RealVector &cv_lower_bnds, const RealVector &cv_upper_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_lower_bnds, const RealVector &lin_ineq_upper_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_targets, const RealVector &nonlin_ineq_lower_bnds, const RealVector &nonlin_ineq_upper_bnds, const RealVector &nonlin_eq_targets, void(∗resp_map)(const Variables &vars, const ActiveSet &set, Response &response)=NULL)

    standard full constructor with minimizer-specific bounds/targets; doubles as a partial constructor given default value for response mapping function pointer
- MinimizerAdapterModel (void(∗resp_map)(const Variables &vars, const ActiveSet &set, Response &response))

    alternate partial constructor; constructs response map but requires subsequent initialize/assign calls
- ∼MinimizerAdapterModel ()

    destructor
- void initialize_variables (size_t num_cdv)

    initialize currentVariables
- void initialize_constraints ()

    initialize userDefinedConstraints
- void initialize_response ()

    initialize currentResponse
- void assign_variables (const RealVector &c_vars)

    assign variable values
- void assign_constraints (const RealVector &cv_lower_bnds, const RealVector &cv_upper_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_lower_bnds, const RealVector &lin_ineq_upper_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_targets, const RealVector &nln_ineq_lower_bnds, const RealVector &nln_ineq_upper_bnds, const RealVector &nln_eq_targets)

    initialize constraint bounds/targets after alternate construction

Additional Inherited Members

14.112.1 Detailed Description

Derived model class which wraps call-back functions for solving minimization sub-problems.

The MinimizerAdapterModel class uses C-style function pointers to: (a) allow use of existing Minimizer constructor APIs that utilize an incoming Model to extract sub-problem data, and (b) enable Model recursions on top of these call-backs.

14.112.2 Constructor & Destructor Documentation

14.112.2.1 MinimizerAdapterModel (const RealVector & *cv_initial_pt,* const RealVector & *cv_lower_bnds,* const RealVector & *cv_upper_bnds,* const RealMatrix & *lin_ineq_coeffs,* const RealVector & *lin_ineq_lower_bnds,* const RealVector & *lin_ineq_upper_bnds,* const RealMatrix & *lin_eq_coeffs,* const RealVector & *lin_eq_targets,* const RealVector & *nonlin_ineq_lower_bnds,* const RealVector & *nonlin_ineq_upper_bnds,* const RealVector & *nonlin_eq_targets,* void(∗)(const **Variables** &vars, const **ActiveSet** &set, **Response** &response) *resp_map =* `NULL`)

standard full constructor with minimizer-specific bounds/targets; doubles as a partial constructor given default value for response mapping function pointer

Default constructor. Includes full definition of a minimization sub-problem.

References MinimizerAdapterModel::assign_constraints(), MinimizerAdapterModel::assign_variables(), Minimizer-AdapterModel::initialize_response(), Model::modelId, and Model::outputLevel.

14.112.2.2 MinimizerAdapterModel (void(∗)(const **Variables** &vars, const **ActiveSet** &set, **Response** &response) *resp_map*)

alternate partial constructor; constructs response map but requires subsequent initialize/assign calls

```
Rely on AdapterModel for this generic case (not Minimizer specific)
```

MinimizerAdapterModel:: MinimizerAdapterModel(const Variables& initial_vars, const Constraints& cons, const Response& resp, void (*resp_map) (const Variables& vars, const ActiveSet& set, Response& response)): Adapter-Model(initial_vars, cons, resp, resp_map) { modelId = "MINIMIZER_ADAPTER"; outputLevel = SILENT_OUTPUT; }This alternate constructor defers initialization of the variable and constraint data until separate calls to initialize_().*

References Model::modelId, and Model::outputLevel.

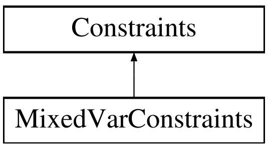
The documentation for this class was generated from the following files:

- MinimizerAdapterModel.hpp
- MinimizerAdapterModel.cpp

14.113 MixedVarConstraints Class Reference

Derived class within the Constraints hierarchy which separates continuous and discrete variables (no domain type array merging).

Inheritance diagram for MixedVarConstraints:



Public Member Functions

- MixedVarConstraints (const SharedVariablesData &svd)

  lightweight constructor
- MixedVarConstraints (const ProblemDescDB &problem_db, const SharedVariablesData &svd)

  standard constructor
- ∼MixedVarConstraints ()

  destructor

- void write (std::ostream &s) const

  write a variable constraints object to an std::ostream
- void read (std::istream &s)

  read a variable constraints object from an std::istream

Additional Inherited Members

14.113.1 Detailed Description

Derived class within the Constraints hierarchy which separates continuous and discrete variables (no domain type array merging).

Derived variable constraints classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The MixedVarConstraints derived class separates the continuous and discrete domain types (see Variables::get_variables(problem_db) for variables type selection; variables type is passed to the Constraints constructor in Model).

14.113.2 Constructor & Destructor Documentation

14.113.2.1 MixedVarConstraints (const ProblemDescDB & *problem_db,* const SharedVariablesData & *svd*)

standard constructor

In this class, mixed continuous/discrete variables are used. Most iterators/strategies use this approach, which is the default in Constraints::get_constraints().

References Constraints::allContinuousLowerBnds, Constraints::allContinuousUpperBnds, Constraints::allDiscreteIntLowerBnds, Constraints::allDiscreteIntUpperBnds, Constraints::allDiscreteRealLowerBnds, Constraints::allDiscreteRealUpperBnds, Dakota::copy_data_partial(), ProblemDescDB::get_iv(), and ProblemDescDB::get_rv().

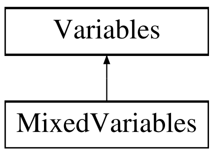
The documentation for this class was generated from the following files:

- MixedVarConstraints.hpp
- MixedVarConstraints.cpp

14.114 MixedVariables Class Reference

Derived class within the Variables hierarchy which separates continuous and discrete variables (no domain type array merging).

Inheritance diagram for MixedVariables:



Public Member Functions

- MixedVariables (const ProblemDescDB &problem_db, const std::pair< short, short > &view)

  standard constructor
- MixedVariables (const SharedVariablesData &svd)

  lightweight constructor

- ∼MixedVariables ()
    destructor

Protected Member Functions

- void read (std::istream &s)
    read a variables object from an std::istream
- void read_tabular (std::istream &s, unsigned short vars_part=ALL_VARS)
- void write (std::ostream &s, unsigned short vars_part=ALL_VARS) const
    write a variables object to an std::ostream, e.g., the console, optionally specifying which partition (all/active/inactive)
- void write_aprepro (std::ostream &s) const
    write a variables object to an std::ostream in aprepro format, e.g., a parameters file
- void write_tabular (std::ostream &s, unsigned short vars_part=ALL_VARS) const
    write a variables object in tabular format to an std::ostream, optionally specifying which partition (all/active/inactive)
- void write_tabular_partial (std::ostream &s, size_t start_index, size_t num_items) const
    write range of variables in tabular format to an std::ostream
- void write_tabular_labels (std::ostream &s, unsigned short vars_part=ALL_VARS) const
    write the labels in input spec order to a std::ostream, optionally specifying which partition (all/active/inactive)
- void write_tabular_partial_labels (std::ostream &s, size_t start_index, size_t num_items) const
    write range of variable labels in input spec order to a std::ostream
- template< typename Reader >
  void read_core (std::istream &s, Reader read_handler, unsigned short vars_part)
    Implementation of reading various formats using the specified read handler.
- template< typename Writer >
  void write_core (std::ostream &s, Writer write_handler, unsigned short vars_part) const
    Implementation for writing various formats using the specified write handler.
- template< typename Writer >
  bool write_partial_core (std::ostream &s, Writer write_handler, size_t start_index, size_t end_index, size_t &acv_offset, size_t &adiv_offset, size_t &adsv_offset, size_t &adrv_offset, size_t &av_cntr, size_t num_cv, size_t num_div, size_t num_dsv, size_t num_drv) const
    Implementation for partial writing in various formats using the specified write handler.

Additional Inherited Members

14.114.1 Detailed Description

Derived class within the Variables hierarchy which separates continuous and discrete variables (no domain type array merging).

Derived variables classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The MixedVariables derived class separates the continuous and discrete domain types (see Variables::get_variables(problem_db)).

14.114.2 Constructor & Destructor Documentation

14.114.2.1 MixedVariables (const ProblemDescDB & *problem_db*, const std::pair< short, short > & *view*)

standard constructor

In this class, the distinct approach is used (design, uncertain, and state variable types and continuous and discrete domain types are distinct). Most iterators/strategies use this approach.

References Variables::allContinuousVars, Variables::allDiscreteIntVars, Variables::allDiscreteRealVars, Variables::allDiscreteStringVars, Dakota::copy_data_partial(), ProblemDescDB::get_iv(), ProblemDescDB::get_rv(), and ProblemDescDB::get_sa().

14.114.3 Member Function Documentation

14.114.3.1 void read_tabular (std::istream & *s,* unsigned short *vars_part* = ALL_VARS) [protected], [virtual]

Tabular reader that reads data in order design, aleatory, epistemic, state according to counts in vc_totals (extract in order: cdv/ddiv/ddrv, cauv/dauiv/daurv, ceuv/deuiv/deurv, csv/dsiv/dsrv, which might reflect active or all depending on context. Assumes container sized, since might be a view into a larger array.

Reimplemented from Variables.

References MixedVariables::read_core().

14.114.3.2 void read_core (std::istream & *s,* Reader *read_handler,* unsigned short *vars_part*) [protected]

Implementation of reading various formats using the specified read handler.

Reordering is required in all read/write cases that will be visible to the user since all derived vars classes should use the same CDV/DDV/UV/CSV/DSV ordering for clarity. Neutral file I/O, binary streams, and packed buffers do not need to reorder (so long as read/write are consistent) since this data is not intended for public consumption.

References SharedVariablesData::active_components_totals(), Variables::all_continuous_variable_labels(), Variables::all_discrete_int_variable_labels(), Variables::all_discrete_real_variable_labels(), Variables::all_discrete_string_variable_labels(), Variables::allContinuousVars, Variables::allDiscreteIntVars, Variables::allDiscreteRealVars, Variables::allDiscreteStringVars, SharedVariablesData::components_totals(), SharedVariablesData::cv_start(), SharedVariablesData::div_start(), SharedVariablesData::drv_start(), SharedVariablesData::dsv_start(), SharedVariablesData::icv_start(), SharedVariablesData::idiv_start(), SharedVariablesData::idrv_start(), SharedVariablesData::idsv_start(), SharedVariablesData::inactive_components_totals(), and Variables::sharedVarsData.

Referenced by MixedVariables::read(), and MixedVariables::read_tabular().

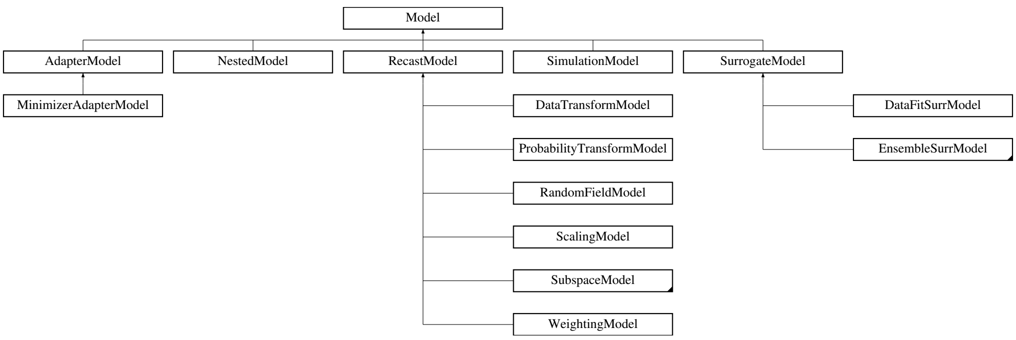
The documentation for this class was generated from the following files:

- MixedVariables.hpp
- MixedVariables.cpp

14.115 Model Class Reference

Base class for the model class hierarchy.

Inheritance diagram for Model:



Public Member Functions

- Model ()

    default constructor

- Model (ProblemDescDB &problem_db)

    standard constructor for envelope
- Model (const Model &model)

    copy constructor
- virtual ∼Model ()

    destructor
- Model operator= (const Model &model)

    assignment operator
- virtual Iterator & subordinate_iterator ()

    return the sub-iterator in nested and surrogate models
- virtual Model & subordinate_model ()

    return a single sub-model defined from subModel in nested and recast models and truth_model() in surrogate models; used for a directed dive through model recursions that may bypass some components.
- virtual void active_model_key (const Pecos::ActiveKey &key)

    set the active model key within surrogate data, grid driver, and approximation classes that support the management of multiple approximation states within surrogate models
- virtual const Pecos::ActiveKey & active_model_key () const

    return the active model key (used by surrogate data, grid driver, and approximation classes to support the management of multiple approximation states within surrogate models)
- virtual void clear_model_keys ()

    reset by removing all model keys within surrogate data, grid driver, and approximation classes that support the management of multiple approximation states within surrogate models
- virtual size_t qoi () const

    return number of unique response functions (managing any aggregations)
- virtual Model & surrogate_model (size_t i=_NPOS)

    return the active approximation sub-model in surrogate models
- virtual const Model & surrogate_model (size_t i=_NPOS) const

    return the active approximation sub-model in surrogate models
- virtual Model & truth_model ()

    return the active truth sub-model in surrogate models
- virtual const Model & truth_model () const

    return the active truth sub-model in surrogate models
- virtual bool multifidelity () const

    identify if hierarchy is across model forms
- virtual bool multilevel () const

    identify if hierarchy is across resolution levels
- virtual bool multilevel_multifidelity () const

    identify if hierarchy is across both model forms and resolution levels
- virtual bool multifidelity_precedence () const

    return precedence for hierarchy definition, model forms or resolution levels
- virtual void multifidelity_precedence (bool mf_prec, bool update_default=false)

    assign precedence for hierarchy definition (model forms or resolution levels) as determined from algorithm context
- virtual void derived_subordinate_models (ModelList &ml, bool recurse_flag)

    portion of subordinate_models() specific to derived model classes
- virtual void resize_from_subordinate_model (size_t depth=SZ_MAX)

    resize vars/resp if needed from the bottom up
- virtual void update_from_subordinate_model (size_t depth=SZ_MAX)

    propagate vars/labels/bounds/targets from the bottom up
- virtual Interface & derived_interface ()

    return the interface employed by the derived model class, if present: SimulationModel::userDefinedInterface, DataFitSurrModel::approxInterface, or NestedModel::optionalInterface
- virtual size_t solution_levels (bool lwr_bnd=true) const

number of discrete levels within solution control (SimulationModel)

- virtual void solution_level_cost_index (size_t index)

  activate a particular level within the solution level control (SimulationModel)
- virtual size_t solution_level_cost_index () const

  return currently active level within the solution level control (SimulationModel)
- virtual RealVector solution_level_costs () const

  return ordered cost estimates across solution levels (SimulationModel)
- virtual Real solution_level_cost () const

  return currently active cost estimate from solution level control (SimulationModel)
- virtual short solution_control_variable_type () const

  return type of solution control variable
- virtual size_t solution_control_variable_index () const

  return index of solution control variable within all variables
- virtual size_t solution_control_discrete_variable_index () const

  return index of solution control variable within all discrete variables
- virtual int solution_level_int_value () const

  return the active (integer) value of the solution control
- virtual String solution_level_string_value () const

  return the active (string) value of the solution control
- virtual Real solution_level_real_value () const

  return the active (real) value of the solution control
- virtual size_t cost_metadata_index () const

  return index of online cost estimates within metadata
- virtual void primary_response_fn_weights (const RealVector &wts, bool recurse_flag=true)

  set the relative weightings for multiple objective functions or least squares terms
- virtual void surrogate_function_indices (const SizetSet &surr_fn_indices)

  set the (currently active) surrogate function index set
- virtual
  Pecos::ProbabilityTransformation & probability_transformation ()

  return probability transformation employed by the Model (forwarded along to ProbabilityTransformModel recasting)
- virtual bool initialize_mapping (ParLevLIter pl_iter)

  Perform any global updates prior to individual evaluate() calls; returns true if the variables size has changed.
- virtual bool finalize_mapping ()

  restore state in preparation for next initialization; returns true if the variables size has changed
- virtual bool resize_pending () const

  return true if a potential resize is still pending, such that sizing-based initialization should be deferred
- virtual void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

  set primaryA{C,DI,DS,DR}VarMapIndices, secondaryA{C,DI,DS,DR}VarMapTargets (coming from a higher-level NestedModel context to inform derivative est.)
- virtual const SizetArray & nested_acv1_indices () const

  return primaryACVarMapIndices
- virtual const ShortArray & nested_acv2_targets () const

  return secondaryACVarMapTargets
- virtual short query_distribution_parameter_derivatives () const

  calculate and return derivative composition of final results w.r.t. distribution parameters (none, all, or mixed)
- virtual void activate_distribution_parameter_derivatives ()

  activate derivative setting w.r.t. distribution parameters
- virtual void deactivate_distribution_parameter_derivatives ()

  deactivate derivative setting w.r.t. distribution parameters

- virtual void trans_grad_X_to_U (const RealVector &fn_grad_x, RealVector &fn_grad_u, const RealVector &x-_vars)

  transform x-space gradient vector to u-space
- virtual void trans_grad_U_to_X (const RealVector &fn_grad_u, RealVector &fn_grad_x, const RealVector &x-_vars)

  transform u-space gradient vector to x-space
- virtual void trans_grad_X_to_S (const RealVector &fn_grad_x, RealVector &fn_grad_s, const RealVector &x-_vars)

  transform x-space gradient vector to gradient with respect to inserted distribution parameters
- virtual void trans_hess_X_to_U (const RealSymMatrix &fn_hess_x, RealSymMatrix &fn_hess_u, const Real-Vector &x_vars, const RealVector &fn_grad_x)

  transform x-space Hessian matrix to u-space
- virtual void build_approximation ()

  build a new SurrogateModel approximation
- virtual bool build_approximation (const Variables &vars, const IntResponsePair &response_pr)

  build a new SurrogateModel approximation using/enforcing anchor response at vars; rebuild if needed
- virtual void rebuild_approximation ()

  incremental rebuild of an existing SurrogateModel approximation
- virtual void rebuild_approximation (const IntResponsePair &response_pr)

  incremental rebuild of an existing SurrogateModel approximation
- virtual void rebuild_approximation (const IntResponseMap &resp_map)

  incremental rebuild of an existing SurrogateModel approximation
- virtual void update_approximation (bool rebuild_flag)

  replace the approximation data within an existing surrogate based on data updates propagated elsewhere
- virtual void update_approximation (const Variables &vars, const IntResponsePair &response_pr, bool rebuild-_flag)

  replace the anchor point data within an existing surrogate
- virtual void update_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)

  replace the data points within an existing surrogate
- virtual void update_approximation (const RealMatrix &samples, const IntResponseMap &resp_map, bool rebuild_flag)

  replace the data points within an existing surrogate
- virtual void append_approximation (bool rebuild_flag)

  append to the existing approximation data within a surrogate based on data updates propagated elsewhere
- virtual void append_approximation (const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)

  append a single point to an existing surrogate's data
- virtual void append_approximation (const RealMatrix &samples, const IntResponseMap &resp_map, bool rebuild_flag)

  append multiple points to an existing surrogate's data
- virtual void append_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)

  append multiple points to an existing surrogate's data
- virtual void append_approximation (const IntVariablesMap &vars_map, const IntResponseMap &resp_map, bool rebuild_flag)

  append multiple points to an existing surrogate's data
- virtual void replace_approximation (const IntResponsePair &response_pr, bool rebuild_flag)

  replace the response for a single point (based on eval id from response_pr) within an existing surrogate's data
- virtual void replace_approximation (const IntResponseMap &resp_map, bool rebuild_flag)

  replace the responses for a set of points (based on eval ids from resp_map) within an existing surrogate's data
- virtual void track_evaluation_ids (bool track)

assigns a flag to track evaluation ids within surrogate data, enabling id-based lookups for data replacement

- virtual void pop_approximation (bool save_surr_data, bool rebuild_flag=false)

  remove the previous data set addition to a surrogate (e.g., due to a previous append_approximation() call); flag manages storing of surrogate data for use in a subsequent push_approximation()
- virtual void push_approximation ()

  push a previous approximation data state; reverse of pop_approximation
- virtual bool push_available ()

  query for whether a trial increment is restorable within a surrogate
- virtual void finalize_approximation ()

  finalize an approximation by applying all previous trial increments
- virtual void combine_approximation ()

  combine the current approximation with previously stored data sets
- virtual void combined_to_active (bool clear_combined=true)

  promote the combined approximation into the active approximation
- virtual void clear_inactive ()

  clear inactive approximations (finalization + combination completed)
- virtual bool advancement_available ()

  query the approximation for available advancement in resolution controls (order, rank, etc.); an input to adaptive refinement strategies
- virtual bool formulation_updated () const

  query the approximation for updates in formulation, requiring a rebuild even if no updates to the build data
- virtual void formulation_updated (bool update)

  assign the status of approximation formulation updates
- virtual void run_dace ()

  execute the DACE iterator (prior to building/appending the approximation)
- virtual bool force_rebuild ()

  determine whether a surrogate model rebuild should be forced based on changes in the inactive data
- virtual SharedApproxData & shared_approximation ()

  retrieve the shared approximation data within the ApproximationInterface of a DataFitSurrModel
- virtual std::vector
  $<$ Approximation $>$ & approximations ()

  retrieve the set of Approximations within the ApproximationInterface of a DataFitSurrModel
- virtual const
  Pecos::SurrogateData & approximation_data (size_t fn_index)

  retrieve a SurrogateData instance from a particular Approximation instance within the ApproximationInterface of a DataFitSurrModel
- virtual const RealVectorArray & approximation_coefficients (bool normalized=false)

  retrieve the approximation coefficients from each Approximation within a DataFitSurrModel
- virtual void approximation_coefficients (const RealVectorArray &approx_coeffs, bool normalized=false)

  set the approximation coefficients for each Approximation within a DataFitSurrModel
- virtual const RealVector & approximation_variances (const Variables &vars)

  retrieve the prediction variances from each Approximation within a DataFitSurrModel
- virtual void surrogate_response_mode (short mode)

  set response computation mode used in SurrogateModels for forming currentResponse
- virtual short surrogate_response_mode () const

  return response computation mode used in SurrogateModels for forming currentResponse
- virtual const RealVector & error_estimates ()

  retrieve error estimates corresponding to the Model's response (could be surrogate error for SurrogateModels, statistical MSE for NestedModels, or adjoint error estimates for SimulationModels). Errors returned correspond to most recent evaluate().
- virtual DiscrepancyCorrection & discrepancy_correction ()

  return the DiscrepancyCorrection object used by SurrogateModels

- virtual void correction_type (short corr_type)

    set the correction type from the DiscrepancyCorrection object used by SurrogateModels
- virtual short correction_type ()

    return the correction type from the DiscrepancyCorrection object used by SurrogateModels
- virtual short correction_order ()

    return the correction order from the DiscrepancyCorrection object used by SurrogateModels
- virtual void single_apply (const Variables &vars, Response &resp, const Pecos::ActiveKey &paired_key)

    apply a DiscrepancyCorrection to correct an approximation within a HierarchSurrModel
- virtual void recursive_apply (const Variables &vars, Response &resp)

    apply a sequence of DiscrepancyCorrections to recursively correct an approximation within a HierarchSurrModel
- virtual void component_parallel_mode (short mode)

    update componentParallelMode for supporting parallelism in model sub-components
- virtual IntIntPair estimate_partition_bounds (int max_eval_concurrency)

    estimate the minimum and maximum partition sizes that can be utilized by this Model
- virtual size_t mi_parallel_level_index () const

    return the index for the metaiterator-iterator parallelism level within ParallelConfiguration::miPLIters that is active for use in a particular Model at runtime
- virtual void cache_unmatched_response (int raw_id)

    migrate an unmatched response record from active response map (computed by synchronize() or synhronize_-nowait()) to cached response map
- virtual void cache_unmatched_responses ()

    migrate remaining response records from responseMap to cachedResponseMap
- virtual short local_eval_synchronization ()

    return derived model synchronization setting
- virtual int local_eval_concurrency ()

    return derived model asynchronous evaluation concurrency
- virtual void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)

    Service job requests received from the master. Completes when a termination message is received from stop_-servers().
- virtual void stop_servers ()

    Executed by the master to terminate all server operations for a particular model when iteration on the model is complete.
- virtual bool derived_master_overload () const

    Return a flag indicating the combination of multiprocessor evaluations and a dedicated master iterator scheduling. Used in synchronous evaluate functions to prevent the error of trying to run a multiprocessor job on the master.
- virtual void create_2d_plots ()

    create 2D graphics plots for automatic logging of vars/response data
- virtual void create_tabular_datastream ()

    create a tabular output stream for automatic logging of vars/response data
- virtual void derived_auto_graphics (const Variables &vars, const Response &resp)

    Update tabular/graphics data with latest variables/response data.
- virtual void inactive_view (short view, bool recurse_flag=true)

    update the Model's inactive view based on higher level (nested) context
- virtual const String & interface_id () const

    return the interface identifier
- virtual int derived_evaluation_id () const

    Return the value of the evaluation id counter for the Model.
- virtual bool evaluation_cache (bool recurse_flag=true) const

    Indicates the usage of an evaluation cache by the Model.
- virtual bool restart_file (bool recurse_flag=true) const

    Indicates the usage of a restart file by the Model.
- virtual void set_evaluation_reference ()

Set the reference points for the evaluation counters within the Model.

- virtual void fine_grained_evaluation_counters ()

  Request fine-grained evaluation reporting within the Model.

- virtual void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_-count=true) const

  Print an evaluation summary for the Model.

- virtual void eval_tag_prefix (const String &eval_id_str)

  set the hierarchical eval ID tag prefix

- virtual bool db_lookup (const Variables &search_vars, const ActiveSet &search_set, Response &found_resp)

  search the eval database (during derivative estimation); derived may need to reimplement due to problem transformations (RecastModel); return true if found in DB

- virtual void stop_init_mapping (ParLevLIter pl_iter)

  called from IteratorScheduler::run_iterator() for iteratorComm rank 0 to terminate serve_init_mapping() on other iteratorComm processors

- virtual int serve_init_mapping (ParLevLIter pl_iter)

  called from IteratorScheduler::run_iterator() for iteratorComm rank != 0 to balance resize() calls on iteratorComm rank 0

- virtual void stop_finalize_mapping (ParLevLIter pl_iter)

  called from IteratorScheduler::run_iterator() for iteratorComm rank 0 to terminate serve_finalize_mapping() on other iteratorComm processors

- virtual int serve_finalize_mapping (ParLevLIter pl_iter)

  called from IteratorScheduler::run_iterator() for iteratorComm rank != 0 to balance resize() calls on iteratorComm rank 0

- virtual void warm_start_flag (const bool flag)

  set the warm start flag (warmStartFlag)

- virtual void declare_sources ()

  Declare a model's sources to the evaluationsDB.

- ModelList & subordinate_models (bool recurse_flag=true)

  return the sub-models in nested and surrogate models

- void evaluate ()

  Compute the Response at currentVariables (default ActiveSet).

- void evaluate (const ActiveSet &set)

  Compute the Response at currentVariables (specified ActiveSet).

- void evaluate_nowait ()

  Spawn an asynchronous job (or jobs) that computes the value of the Response at currentVariables (default ActiveSet).

- void evaluate_nowait (const ActiveSet &set)

  Spawn an asynchronous job (or jobs) that computes the value of the Response at currentVariables (specified ActiveSet).

- const IntResponseMap & synchronize ()

  Execute a blocking scheduling algorithm to collect the complete set of results from a group of asynchronous evaluations.

- const IntResponseMap & synchronize_nowait ()

  Execute a nonblocking scheduling algorithm to collect all available results from a group of asynchronous evaluations.

- int evaluation_id () const

  return Model's (top-level) evaluation counter, not to be confused with derived counter returned by derived_evaluation_id()

- bool **mapping_initialized** () const
- void init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  allocate communicator partitions for a model and store configuration in modelPCIterMap

- void init_serial ()

  for cases where init_communicators() will not be called, modify some default settings to behave properly in serial.

- void set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true) *set active parallel configuration for the model (set modelPCIter from modelPCIterMap)*

- void free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  deallocate communicator partitions for a model
- MPI_Comm analysis_comm () const

  retrieve the MPI communicator on which this model is configured to conduct function evaluation analyses (provided for library clients)
- void stop_init_communicators (ParLevLIter pl_iter)

  called from IteratorScheduler::init_iterator() for iteratorComm rank 0 to terminate serve_init_communicators() on other iteratorComm processors
- int serve_init_communicators (ParLevLIter pl_iter)

  called from IteratorScheduler::init_iterator() for iteratorComm rank != 0 to balance init_communicators() calls on iteratorComm rank 0
- void estimate_message_lengths ()

  estimate messageLengths for a model
- size_t response_size () const

  return (potentially aggregated) size of response vector in currentResponse
- bool manage_data_recastings ()

  initialize modelList and recastFlags for data import/export
- bool recastings () const

  return true if recastFlags is defined
- void user_space_to_iterator_space (const Variables &user_vars, const Response &user_resp, Variables &iter_vars, Response &iter_resp)

  employ the model recursion to transform from bottom level user-space data to top level iterator-space data
- void iterator_space_to_user_space (const Variables &iter_vars, const Response &iter_resp, Variables &user_vars, Response &user_resp)

  employ the model recursion to transform from top level iterator-space data to bottom level user-space data
- void assign_rep (std::shared_ptr< Model > model_rep)

  replaces existing letter with a new one
- size_t tv () const

  returns total number of vars
- size_t cv () const

  returns number of active continuous variables
- size_t div () const

  returns number of active discrete integer vars
- size_t dsv () const

  returns number of active discrete string vars
- size_t drv () const

  returns number of active discrete real vars
- size_t icv () const

  returns number of inactive continuous variables
- size_t idiv () const

  returns number of inactive discrete integer vars
- size_t idsv () const

  returns number of inactive discrete string vars
- size_t idrv () const

  returns number of inactive discrete real vars
- size_t acv () const

  returns total number of continuous variables
- size_t adiv () const

  returns total number of discrete integer vars
- size_t adsv () const

returns total number of discrete string vars
- size_t adrv () const

  returns total number of discrete real vars
- void active_variables (const Variables &vars)

  set the active variables in currentVariables
- void inactive_variables (const Variables &vars)

  set the inactive variables in currentVariables
- const RealVector & continuous_variables () const

  return the active continuous variables from currentVariables
- Real continuous_variable (size_t i) const

  return an active continuous variable from currentVariables
- void continuous_variables (const RealVector &c_vars)

  set the active continuous variables in currentVariables
- void continuous_variable (Real c_var, size_t i)

  set an active continuous variable in currentVariables
- const IntVector & discrete_int_variables () const

  return the active discrete integer variables from currentVariables
- int discrete_int_variable (size_t i) const

  return an active discrete integer variable from currentVariables
- void discrete_int_variables (const IntVector &d_vars)

  set the active discrete integer variables in currentVariables
- void discrete_int_variable (int d_var, size_t i)

  set an active discrete integer variable in currentVariables
- StringMultiArrayConstView discrete_string_variables () const

  return the active discrete string variables from currentVariables
- const String & discrete_string_variable (size_t i) const

  return an active discrete string variable from currentVariables
- void discrete_string_variables (StringMultiArrayConstView d_vars)

  set the active discrete string variables in currentVariables
- void discrete_string_variable (const String &d_var, size_t i)

  set an active discrete string variable in currentVariables
- const RealVector & discrete_real_variables () const

  return the active discrete real variables from currentVariables
- Real discrete_real_variable (size_t i) const

  return an active discrete real variable from currentVariables
- void discrete_real_variables (const RealVector &d_vars)

  set the active discrete real variables in currentVariables
- void discrete_real_variable (Real d_var, size_t i)

  set an active discrete real variable in currentVariables
- UShortMultiArrayConstView continuous_variable_types () const

  return the active continuous variable types from currentVariables
- void continuous_variable_types (UShortMultiArrayConstView cv_types)

  set the active continuous variable types in currentVariables
- void continuous_variable_type (unsigned short cv_type, size_t i)

  set an active continuous variable type in currentVariables
- UShortMultiArrayConstView discrete_int_variable_types () const

  return the active discrete variable types from currentVariables
- void discrete_int_variable_types (UShortMultiArrayConstView div_types)

  set the active discrete variable types in currentVariables
- void discrete_int_variable_type (unsigned short div_type, size_t i)

  set an active discrete variable type in currentVariables

- UShortMultiArrayConstView discrete_string_variable_types () const

    return the active discrete variable types from currentVariables
- void discrete_string_variable_types (UShortMultiArrayConstView div_types)

    set the active discrete variable types in currentVariables
- void discrete_string_variable_type (unsigned short div_type, size_t i)

    set an active discrete variable type in currentVariables
- UShortMultiArrayConstView discrete_real_variable_types () const

    return the active discrete variable types from currentVariables
- void discrete_real_variable_types (UShortMultiArrayConstView drv_types)

    set the active discrete variable types in currentVariables
- void discrete_real_variable_type (unsigned short drv_type, size_t i)

    set an active discrete variable type in currentVariables
- SizetMultiArrayConstView continuous_variable_ids () const

    return the active continuous variable identifiers from currentVariables
- void continuous_variable_ids (SizetMultiArrayConstView cv_ids)

    set the active continuous variable identifiers in currentVariables
- void continuous_variable_id (size_t cv_id, size_t i)

    set an active continuous variable identifier in currentVariables
- const RealVector & inactive_continuous_variables () const

    return the inactive continuous variables in currentVariables
- void inactive_continuous_variables (const RealVector &i_c_vars)

    set the inactive continuous variables in currentVariables
- const IntVector & inactive_discrete_int_variables () const

    return the inactive discrete variables in currentVariables
- void inactive_discrete_int_variables (const IntVector &i_d_vars)

    set the inactive discrete variables in currentVariables
- StringMultiArrayConstView inactive_discrete_string_variables () const

    return the inactive discrete variables in currentVariables
- void inactive_discrete_string_variables (StringMultiArrayConstView i_d_vars)

    set the inactive discrete variables in currentVariables
- const RealVector & inactive_discrete_real_variables () const

    return the inactive discrete variables in currentVariables
- void inactive_discrete_real_variables (const RealVector &i_d_vars)

    set the inactive discrete variables in currentVariables
- UShortMultiArrayConstView inactive_continuous_variable_types () const

    return the inactive continuous variable types from currentVariables
- SizetMultiArrayConstView inactive_continuous_variable_ids () const

    return the inactive continuous variable identifiers from currentVariables
- const RealVector & all_continuous_variables () const

    return all continuous variables in currentVariables
- void all_continuous_variables (const RealVector &a_c_vars)

    set all continuous variables in currentVariables
- void all_continuous_variable (Real a_c_var, size_t i)

    set a variable within the all continuous variables in currentVariables
- const IntVector & all_discrete_int_variables () const

    return all discrete variables in currentVariables
- void all_discrete_int_variables (const IntVector &a_d_vars)

    set all discrete variables in currentVariables
- void all_discrete_int_variable (int a_d_var, size_t i)

    set a variable within the all discrete variables in currentVariables
- StringMultiArrayConstView all_discrete_string_variables () const

return all discrete variables in currentVariables

- void all_discrete_string_variables (StringMultiArrayConstView a_d_vars)

  set all discrete variables in currentVariables
- void all_discrete_string_variable (const String &a_d_var, size_t i)

  set a variable within the all discrete variables in currentVariables
- const RealVector & all_discrete_real_variables () const

  return all discrete variables in currentVariables
- void all_discrete_real_variables (const RealVector &a_d_vars)

  set all discrete variables in currentVariables
- void all_discrete_real_variable (Real a_d_var, size_t i)

  set a variable within the all discrete variables in currentVariables
- UShortMultiArrayConstView all_continuous_variable_types () const

  return all continuous variable types from currentVariables
- UShortMultiArrayConstView all_discrete_int_variable_types () const

  return all discrete variable types from currentVariables
- UShortMultiArrayConstView all_discrete_string_variable_types () const

  return all discrete variable types from currentVariables
- UShortMultiArrayConstView all_discrete_real_variable_types () const

  return all discrete variable types from currentVariables
- SizetMultiArrayConstView all_continuous_variable_ids () const

  return all continuous variable identifiers from currentVariables
- const BitArray & discrete_int_sets ()

  define and return discreteIntSets using active view from currentVariables
- const BitArray & discrete_int_sets (short active_view)

  define and return discreteIntSets using passed active view
- const IntSetArray & discrete_set_int_values ()

  return the sets of values available for each of the active discrete set integer variables (aggregated in activeDiscSetIntValues)
- const IntSetArray & discrete_set_int_values (short active_view)

  return the sets of values available for each of the active discrete set integer variables (aggregated in activeDiscSetIntValues)
- const StringSetArray & discrete_set_string_values ()

  return the sets of values available for each of the active discrete set string variables (aggregated in activeDiscSetStringValues)
- const StringSetArray & discrete_set_string_values (short active_view)

  return the sets of values available for each of the active discrete set string variables (aggregated in activeDiscSetStringValues)
- const RealSetArray & discrete_set_real_values ()

  return the sets of values available for each of the active discrete set real variables (aggregated in activeDiscSetRealValues)
- const RealSetArray & discrete_set_real_values (short active_view)

  return the sets of values available for each of the active discrete set real variables (aggregated in activeDiscSetRealValues)
- Pecos::MultivariateDistribution & multivariate_distribution ()

  return mvDist
- const
  Pecos::MultivariateDistribution & multivariate_distribution () const

  return mvDist
- StringMultiArrayConstView continuous_variable_labels () const

  return the active continuous variable labels from currentVariables
- void continuous_variable_labels (StringMultiArrayConstView c_v_labels)

  set the active continuous variable labels in currentVariables

- StringMultiArrayConstView discrete_int_variable_labels () const
  return the active discrete variable labels from currentVariables
- void discrete_int_variable_labels (StringMultiArrayConstView d_v_labels)
  set the active discrete variable labels in currentVariables
- StringMultiArrayConstView discrete_string_variable_labels () const
  return the active discrete variable labels from currentVariables
- void discrete_string_variable_labels (StringMultiArrayConstView d_v_labels)
  set the active discrete variable labels in currentVariables
- StringMultiArrayConstView discrete_real_variable_labels () const
  return the active discrete variable labels from currentVariables
- void discrete_real_variable_labels (StringMultiArrayConstView d_v_labels)
  set the active discrete variable labels in currentVariables
- StringMultiArrayConstView inactive_continuous_variable_labels () const
  return the inactive continuous variable labels in currentVariables
- void inactive_continuous_variable_labels (StringMultiArrayConstView i_c_v_labels)
  set the inactive continuous variable labels in currentVariables
- StringMultiArrayConstView inactive_discrete_int_variable_labels () const
  return the inactive discrete variable labels in currentVariables
- void inactive_discrete_int_variable_labels (StringMultiArrayConstView i_d_v_labels)
  set the inactive discrete variable labels in currentVariables
- StringMultiArrayConstView inactive_discrete_string_variable_labels () const
  return the inactive discrete variable labels in currentVariables
- void inactive_discrete_string_variable_labels (StringMultiArrayConstView i_d_v_labels)
  set the inactive discrete variable labels in currentVariables
- StringMultiArrayConstView inactive_discrete_real_variable_labels () const
  return the inactive discrete variable labels in currentVariables
- void inactive_discrete_real_variable_labels (StringMultiArrayConstView i_d_v_labels)
  set the inactive discrete variable labels in currentVariables
- StringMultiArrayConstView all_continuous_variable_labels () const
  return all continuous variable labels in currentVariables
- void all_continuous_variable_labels (StringMultiArrayConstView a_c_v_labels)
  set all continuous variable labels in currentVariables
- void all_continuous_variable_label (const String &a_c_v_label, size_t i)
  set a label within the all continuous labels in currentVariables
- StringMultiArrayConstView all_discrete_int_variable_labels () const
  return all discrete variable labels in currentVariables
- void all_discrete_int_variable_labels (StringMultiArrayConstView a_d_v_labels)
  set all discrete variable labels in currentVariables
- void all_discrete_int_variable_label (const String &a_d_v_label, size_t i)
  set a label within the all discrete labels in currentVariables
- StringMultiArrayConstView all_discrete_string_variable_labels () const
  return all discrete variable labels in currentVariables
- void all_discrete_string_variable_labels (StringMultiArrayConstView a_d_v_labels)
  set all discrete variable labels in currentVariables
- void all_discrete_string_variable_label (const String &a_d_v_label, size_t i)
  set a label within the all discrete labels in currentVariables
- StringMultiArrayConstView all_discrete_real_variable_labels () const
  return all discrete variable labels in currentVariables
- void all_discrete_real_variable_labels (StringMultiArrayConstView a_d_v_labels)
  set all discrete variable labels in currentVariables
- void all_discrete_real_variable_label (const String &a_d_v_label, size_t i)

set a label within the all discrete labels in currentVariables
- const StringArray & response_labels () const

  return the response labels from currentResponse
- void response_labels (const StringArray &resp_labels)

  set the response labels in currentResponse
- const RealVector & continuous_lower_bounds () const

  return the active continuous lower bounds from userDefinedConstraints
- Real continuous_lower_bound (size_t i) const

  return an active continuous lower bound from userDefinedConstraints
- void continuous_lower_bounds (const RealVector &c_l_bnds)

  set the active continuous lower bounds in userDefinedConstraints
- void continuous_lower_bound (Real c_l_bnd, size_t i)

  set the i-th active continuous lower bound in userDefinedConstraints
- const RealVector & continuous_upper_bounds () const

  return the active continuous upper bounds from userDefinedConstraints
- Real continuous_upper_bound (size_t i) const

  return an active continuous upper bound from userDefinedConstraints
- void continuous_upper_bounds (const RealVector &c_u_bnds)

  set the active continuous upper bounds in userDefinedConstraints
- void continuous_upper_bound (Real c_u_bnd, size_t i)

  set the i-th active continuous upper bound from userDefinedConstraints
- const IntVector & discrete_int_lower_bounds () const

  return the active discrete int lower bounds from userDefinedConstraints
- int discrete_int_lower_bound (size_t i) const

  return an active discrete int lower bound from userDefinedConstraints
- void discrete_int_lower_bounds (const IntVector &d_l_bnds)

  set the active discrete int lower bounds in userDefinedConstraints
- void discrete_int_lower_bound (int d_l_bnd, size_t i)

  set the i-th active discrete int lower bound in userDefinedConstraints
- const IntVector & discrete_int_upper_bounds () const

  return the active discrete int upper bounds from userDefinedConstraints
- int discrete_int_upper_bound (size_t i) const

  return an active discrete int upper bound from userDefinedConstraints
- void discrete_int_upper_bounds (const IntVector &d_u_bnds)

  set the active discrete int upper bounds in userDefinedConstraints
- void discrete_int_upper_bound (int d_u_bnd, size_t i)

  set the i-th active discrete int upper bound in userDefinedConstraints
- const RealVector & discrete_real_lower_bounds () const

  return the active discrete real lower bounds from userDefinedConstraints
- Real discrete_real_lower_bound (size_t i) const

  return an active discrete real lower bound from userDefinedConstraints
- void discrete_real_lower_bounds (const RealVector &d_l_bnds)

  set the active discrete real lower bounds in userDefinedConstraints
- void discrete_real_lower_bound (Real d_l_bnd, size_t i)

  set the i-th active discrete real lower bound in userDefinedConstraints
- const RealVector & discrete_real_upper_bounds () const

  return the active discrete real upper bounds from userDefinedConstraints
- Real discrete_real_upper_bound (size_t i) const

  return an active discrete real upper bound from userDefinedConstraints
- void discrete_real_upper_bounds (const RealVector &d_u_bnds)

  set the active discrete real upper bounds in userDefinedConstraints

- void discrete_real_upper_bound (Real d_u_bnd, size_t i)
  set the i-th active discrete real upper bound in userDefinedConstraints
- const RealVector & inactive_continuous_lower_bounds () const
  return the inactive continuous lower bounds in userDefinedConstraints
- void inactive_continuous_lower_bounds (const RealVector &i_c_l_bnds)
  set the inactive continuous lower bounds in userDefinedConstraints
- const RealVector & inactive_continuous_upper_bounds () const
  return the inactive continuous upper bounds in userDefinedConstraints
- void inactive_continuous_upper_bounds (const RealVector &i_c_u_bnds)
  set the inactive continuous upper bounds in userDefinedConstraints
- const IntVector & inactive_discrete_int_lower_bounds () const
  return the inactive discrete lower bounds in userDefinedConstraints
- void inactive_discrete_int_lower_bounds (const IntVector &i_d_l_bnds)
  set the inactive discrete lower bounds in userDefinedConstraints
- const IntVector & inactive_discrete_int_upper_bounds () const
  return the inactive discrete upper bounds in userDefinedConstraints
- void inactive_discrete_int_upper_bounds (const IntVector &i_d_u_bnds)
  set the inactive discrete upper bounds in userDefinedConstraints
- const RealVector & inactive_discrete_real_lower_bounds () const
  return the inactive discrete lower bounds in userDefinedConstraints
- void inactive_discrete_real_lower_bounds (const RealVector &i_d_l_bnds)
  set the inactive discrete lower bounds in userDefinedConstraints
- const RealVector & inactive_discrete_real_upper_bounds () const
  return the inactive discrete upper bounds in userDefinedConstraints
- void inactive_discrete_real_upper_bounds (const RealVector &i_d_u_bnds)
  set the inactive discrete upper bounds in userDefinedConstraints
- const RealVector & all_continuous_lower_bounds () const
  return all continuous lower bounds in userDefinedConstraints
- void all_continuous_lower_bounds (const RealVector &a_c_l_bnds)
  set all continuous lower bounds in userDefinedConstraints
- void all_continuous_lower_bound (Real a_c_l_bnd, size_t i)
  set a lower bound within continuous lower bounds in userDefinedConstraints
- const RealVector & all_continuous_upper_bounds () const
  return all continuous upper bounds in userDefinedConstraints
- void all_continuous_upper_bounds (const RealVector &a_c_u_bnds)
  set all continuous upper bounds in userDefinedConstraints
- void all_continuous_upper_bound (Real a_c_u_bnd, size_t i)
  set an upper bound within all continuous upper bounds in userDefinedConstraints
- const IntVector & all_discrete_int_lower_bounds () const
  return all discrete lower bounds in userDefinedConstraints
- void all_discrete_int_lower_bounds (const IntVector &a_d_l_bnds)
  set all discrete lower bounds in userDefinedConstraints
- void all_discrete_int_lower_bound (int a_d_l_bnd, size_t i)
  set a lower bound within all discrete lower bounds in userDefinedConstraints
- const IntVector & all_discrete_int_upper_bounds () const
  return all discrete upper bounds in userDefinedConstraints
- void all_discrete_int_upper_bounds (const IntVector &a_d_u_bnds)
  set all discrete upper bounds in userDefinedConstraints
- void all_discrete_int_upper_bound (int a_d_u_bnd, size_t i)
  set an upper bound within all discrete upper bounds in userDefinedConstraints
- const RealVector & all_discrete_real_lower_bounds () const

return all discrete lower bounds in userDefinedConstraints
- void all_discrete_real_lower_bounds (const RealVector &a_d_l_bnds)

  set all discrete lower bounds in userDefinedConstraints
- void all_discrete_real_lower_bound (Real a_d_l_bnd, size_t i)

  set a lower bound within all discrete lower bounds in userDefinedConstraints
- const RealVector & all_discrete_real_upper_bounds () const

  return all discrete upper bounds in userDefinedConstraints
- void all_discrete_real_upper_bounds (const RealVector &a_d_u_bnds)

  set all discrete upper bounds in userDefinedConstraints
- void all_discrete_real_upper_bound (Real a_d_u_bnd, size_t i)

  set an upper bound within all discrete upper bounds in userDefinedConstraints
- void reshape_constraints (size_t num_nln_ineq_cons, size_t num_nln_eq_cons, size_t num_lin_ineq_cons, size_t num_lin_eq_cons)

  reshape the linear/nonlinear constraint arrays
- size_t num_linear_ineq_constraints () const

  return the number of linear inequality constraints
- size_t num_linear_eq_constraints () const

  return the number of linear equality constraints
- const RealMatrix & linear_ineq_constraint_coeffs () const

  return the linear inequality constraint coefficients
- void linear_ineq_constraint_coeffs (const RealMatrix &lin_ineq_coeffs)

  set the linear inequality constraint coefficients
- const RealVector & linear_ineq_constraint_lower_bounds () const

  return the linear inequality constraint lower bounds
- void linear_ineq_constraint_lower_bounds (const RealVector &lin_ineq_l_bnds)

  set the linear inequality constraint lower bounds
- const RealVector & linear_ineq_constraint_upper_bounds () const

  return the linear inequality constraint upper bounds
- void linear_ineq_constraint_upper_bounds (const RealVector &lin_ineq_u_bnds)

  set the linear inequality constraint upper bounds
- const RealMatrix & linear_eq_constraint_coeffs () const

  return the linear equality constraint coefficients
- void linear_eq_constraint_coeffs (const RealMatrix &lin_eq_coeffs)

  set the linear equality constraint coefficients
- const RealVector & linear_eq_constraint_targets () const

  return the linear equality constraint targets
- void linear_eq_constraint_targets (const RealVector &lin_eq_targets)

  set the linear equality constraint targets
- size_t num_nonlinear_ineq_constraints () const

  return the number of nonlinear inequality constraints
- size_t num_nonlinear_eq_constraints () const

  return the number of nonlinear equality constraints
- const RealVector & nonlinear_ineq_constraint_lower_bounds () const

  return the nonlinear inequality constraint lower bounds
- void nonlinear_ineq_constraint_lower_bounds (const RealVector &nln_ineq_l_bnds)

  set the nonlinear inequality constraint lower bounds
- const RealVector & nonlinear_ineq_constraint_upper_bounds () const

  return the nonlinear inequality constraint upper bounds
- void nonlinear_ineq_constraint_upper_bounds (const RealVector &nln_ineq_u_bnds)

  set the nonlinear inequality constraint upper bounds
- const RealVector & nonlinear_eq_constraint_targets () const

return the nonlinear equality constraint targets
- void nonlinear_eq_constraint_targets (const RealVector &nln_eq_targets)

  set the nonlinear equality constraint targets
- const Variables & current_variables () const

  return the current variables (currentVariables) as const reference (preferred)
- Variables & current_variables ()

  return the current variables (currentVariables) in mutable form (special cases)
- const Constraints & user_defined_constraints () const

  return the user-defined constraints (userDefinedConstraints)
- const Response & current_response () const

  return the current response (currentResponse)
- ProblemDescDB & problem_description_db () const

  return the problem description database (probDescDB)
- ParallelLibrary & parallel_library () const

  return the parallel library (parallelLib)
- const String & model_type () const

  return the model type (modelType)
- const String & surrogate_type () const

  return the surrogate type (surrogateType)
- const String & model_id () const

  return the model identifier (modelId)
- size_t num_primary_fns () const

  return number of primary functions (total less nonlinear constraints)
- size_t num_secondary_fns () const

  return number of secondary functions (number of nonlinear constraints)
- const String & gradient_type () const

  return the gradient evaluation type (gradientType)
- const String & method_source () const

  return the numerical gradient evaluation method source (methodSource)
- const String & interval_type () const

  return the numerical gradient evaluation interval type (intervalType)
- bool ignore_bounds () const

  option for ignoring bounds when numerically estimating derivatives
- bool central_hess () const

  option for using old 2nd-order scheme when computing finite-diff Hessian
- const RealVector & fd_gradient_step_size () const

  return the finite difference gradient step size (fdGradStepSize)
- const String & fd_gradient_step_type () const

  return the finite difference gradient step type (fdGradStepType)
- const IntSet & gradient_id_analytic () const

  return the mixed gradient analytic IDs (gradIdAnalytic)
- const IntSet & gradient_id_numerical () const

  return the mixed gradient numerical IDs (gradIdNumerical)
- const String & hessian_type () const

  return the Hessian evaluation type (hessianType)
- const String & quasi_hessian_type () const

  return the Hessian evaluation type (quasiHessType)
- const RealVector & fd_hessian_by_grad_step_size () const

  return gradient-based finite difference Hessian step size (fdHessByGradStepSize)
- const RealVector & fd_hessian_by_fn_step_size () const

  return function-based finite difference Hessian step size (fdHessByFnStepSize)

- const String & fd_hessian_step_type () const

  return the finite difference Hessian step type (fdHessStepType)
- const IntSet & hessian_id_analytic () const

  return the mixed Hessian analytic IDs (hessIdAnalytic)
- const IntSet & hessian_id_numerical () const

  return the mixed Hessian analytic IDs (hessIdNumerical)
- const IntSet & hessian_id_quasi () const

  return the mixed Hessian analytic IDs (hessIdQuasi)
- void primary_response_fn_sense (const BoolDeque &sense)

  set the optimization sense for multiple objective functions
- const BoolDeque & primary_response_fn_sense () const

  get the optimization sense for multiple objective functions
- const RealVector & primary_response_fn_weights () const

  get the relative weightings for multiple objective functions or least squares terms
- const ScalingOptions & scaling_options () const

  user-provided scaling options
- short primary_fn_type () const

  get the primary response function type (generic, objective, calibration)
- void primary_fn_type (short type)

  set the primary response function type, e.g., when recasting
- bool derivative_estimation ()

  indicates potential usage of estimate_derivatives() based on gradientType/hessianType
- void supports_derivative_estimation (bool sed_flag)

  set whether this model should perform or pass on derivative estimation
- void init_comms_bcast_flag (bool icb_flag)

  set initCommsBcastFlag
- int evaluation_capacity () const

  return the evaluation capacity for use in iterator logic
- int derivative_concurrency () const

  return the gradient concurrency for use in parallel configuration logic
- bool asynch_flag () const

  return the asynchronous evaluation flag (asynchEvalFlag)
- void asynch_flag (const bool flag)

  set the asynchronous evaluation flag (asynchEvalFlag)
- short output_level () const

  return the outputLevel
- void output_level (const short level)

  set the outputLevel
- const IntArray & message_lengths () const

  return the array of MPI packed message buffer lengths (messageLengths)
- void parallel_configuration_iterator (ParConfigLIter pc_iter)

  set modelPCIter
- ParConfigLIter parallel_configuration_iterator () const

  return modelPCIter
- void auto_graphics (const bool flag)

  set modelAutoGraphicsFlag to activate posting of graphics data within evaluate/synchronize functions (automatic graphics posting in the model as opposed to graphics posting at the strategy level).
- bool auto_graphics () const

  get modelAutoGraphicsFlag to activate posting of graphics data within evaluate/synchronize functions (automatic graphics posting in the model as opposed to graphics posting at the strategy level).
- bool is_null () const

function to check modelRep (does this envelope contain a letter)

- std::shared_ptr< Model > model_rep () const

    returns modelRep for access to derived class member functions that are not mapped to the top Model level

- virtual String root_model_id ()

    Return the model ID of the "innermost" model. For all derived Models except RecastModels, return modelId. The RecastModel override returns the root_model_id() of the subModel.

- virtual ActiveSet **default_active_set** ()

Static Public Member Functions

- static void active_variables (const RealVector &config_vars, Model &model)

    set the specified configuration to the Model's inactive vars, converting from real to integer or through index to string value as needed

- static void inactive_variables (const RealVector &config_vars, Model &model)

    set the specified configuration to the Model's inactive vars, converting from real to integer or through index to string value as needed

- static void inactive_variables (const RealVector &config_vars, Model &model, Variables &updated_vars)
- static void evaluate (const RealMatrix &samples_matrix, Model &model, RealMatrix &resp_matrix)

    Bulk synchronously evaluate the model for each column (of active variables) in the samples matrix and return as columns of the response matrix.

- static void evaluate (const VariablesArray &sample_vars, Model &model, RealMatrix &resp_matrix)

    Bulk synchronously evaluate the model for each entry (of active variables) in the samples vector and return as columns of the response matrix.

Protected Member Functions

- Model (BaseConstructor, ProblemDescDB &problem_db)

    constructor initializing the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

- Model (LightWtBaseConstructor, const SharedVariablesData &svd, bool share_svd, const SharedResponse-Data &srd, bool share_srd, const ActiveSet &set, short output_level, ProblemDescDB &problem_db=dummy-_db, ParallelLibrary &parallel_lib=dummy_lib)

    constructor initializing base class for derived model class instances constructed on the fly

- Model (LightWtBaseConstructor, ProblemDescDB &problem_db=dummy_db, ParallelLibrary &parallel_-lib=dummy_lib)

    constructor initializing base class for recast model instances

- virtual void derived_evaluate (const ActiveSet &set)

    portion of evaluate() specific to derived model classes

- virtual void derived_evaluate_nowait (const ActiveSet &set)

    portion of evaluate_nowait() specific to derived model classes

- virtual const IntResponseMap & derived_synchronize ()

    portion of synchronize() specific to derived model classes

- virtual const IntResponseMap & derived_synchronize_nowait ()

    portion of synchronize_nowait() specific to derived model classes

- virtual void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_-flag=true)

    portion of init_communicators() specific to derived model classes

- virtual void derived_init_serial ()

    portion of init_serial() specific to derived model classes

- virtual void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_-flag=true)

    portion of set_communicators() specific to derived model classes

- virtual void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_-flag=true)

  portion of free_communicators() specific to derived model classes
- IntResponseMap & response_map ()

  return responseMap
- void initialize_distribution (Pecos::MultivariateDistribution &mv_dist, bool active_only=false)

  initialize distribution types from problemDescDB
- void initialize_distribution_parameters (Pecos::MultivariateDistribution &mv_dist, bool active_only=false)

  initialize distribution parameters from problemDescDB
- void set_ie_asynchronous_mode (int max_eval_concurrency)

  default logic for defining asynchEvalFlag and evaluationCapacity based on ie_pl settings
- void assign_max_strings (const Pecos::MultivariateDistribution &mv_dist, Variables &vars)

  assign all of the longest possible string values into vars
- SSCIter max_string (const StringSet &ss)

  return iterator for longest string value found in string set
- SRMCIter max_string (const StringRealMap &srm)

  return iterator for longest string value found in string map
- SizetMultiArrayConstView initialize_x0_bounds (const SizetArray &original_dvv, bool &active_derivs, bool &inactive_derivs, RealVector &x0, RealVector &fd_lb, RealVector &fd_ub) const

  Initialize data needed for computing finite differences (active/inactive, center point, and bounds)
- Real forward_grad_step (size_t num_deriv_vars, size_t xj_index, Real x0_j, Real lb_j, Real ub_j)

  Compute the forward step for a finite difference gradient; updates shortStep.
- EvaluationsDBState evaluations_db_state (const Interface &interface)

  Return the interface flag for the EvaluationsDB state.
- EvaluationsDBState evaluations_db_state (const Model &model)

  Return the model flag for the EvaluationsDB state.
- void asynch_eval_store (const Interface &interface, const int &id, const Response &response)

  Store the response portion of an interface evaluation. Called from rekey_response_map()
- void asynch_eval_store (const Model &model, const int &id, const Response &response)

  Exists to support storage of interface evaluations. No-op so that rekey_response_map<Model> can be generated.
- template<typename MetaType >
  void rekey_response_map (MetaType &meta_object, IntIntMapArray &id_maps, IntResponseMapArray &resp_maps_rekey, bool deep_copy)

  rekey returned jobs matched in array of id_maps into array of resp_maps_rekey; unmatched jobs can be cached within the meta_object
- template<typename MetaType >
  void rekey_response_map (MetaType &meta_object, IntIntMap &id_map, IntResponseMap &resp_map_-rekey, bool deep_copy)

  rekey returned jobs matched in id_map into resp_map_rekey; unmatched jobs can be cached within the meta_object
- template<typename MetaType >
  void rekey_synch (MetaType &meta_object, bool block, IntIntMapArray &id_maps, IntResponseMapArray &resp_maps_rekey, bool deep_copy=false)

  synchronize via meta_object and rekey returned jobs matched in array of id_maps into array of resp_maps_rekey; unmatched jobs are cached within the meta_object
- template<typename MetaType >
  void rekey_synch (MetaType &meta_object, bool block, IntIntMap &id_map, IntResponseMap &resp_map_-rekey, bool deep_copy=false)

  synchronize via meta_object and rekey returned jobs matched in id_map into resp_map_rekey; unmatched jobs are cached within the meta_object

Static Protected Member Functions

- static String user_auto_id ()

  return the next available model ID for no-ID user methods
- static String no_spec_id ()

  return the next available model ID for on-the-fly methods

Protected Attributes

- Variables currentVariables

  the set of current variables used by the model for performing function evaluations
- size_t numDerivVars

  the number of active continuous variables used in computing most response derivatives (i.e., in places such as quasi-Hessians and response corrections where only the active continuous variables are supported)
- Response currentResponse

  the set of current responses that holds the results of model function evaluations
- size_t numFns

  the number of functions in currentResponse
- Constraints userDefinedConstraints

  Explicit constraints on variables are maintained in the Constraints class hierarchy. Currently, this includes linear constraints and bounds, but could be extended in the future to include other explicit constraints which (1) have their form specified by the user, and (2) are not catalogued in Response since their form and coefficients are published to an iterator at startup.
- String modelId

  model identifier string from the input file
- String modelType

  type of model: simulation, nested, or surrogate
- String surrogateType

  type of surrogate model: local_∗, multipoint_∗, global_∗, or hierarchical
- String gradientType

  type of gradient data: analytic, numerical, mixed, or none
- String methodSource

  source of numerical gradient routine: dakota or vendor
- String intervalType

  type of numerical gradient interval: central or forward
- String hessianType

  type of Hessian data: analytic, numerical, quasi, mixed, or none
- RealVector fdGradStepSize

  relative finite difference step size for numerical gradients
- String fdGradStepType

  type of finite difference step to use for numerical gradient: relative - step length is relative to x absolute - step length is what is specified bounds - step length is relative to range of x
- RealVector fdHessByGradStepSize

  relative finite difference step size for numerical Hessians estimated using first-order differences of gradients
- RealVector fdHessByFnStepSize

  relative finite difference step size for numerical Hessians estimated using second-order differences of function values
- String fdHessStepType

  type of finite difference step to use for numerical Hessian: relative - step length is relative to x absolute - step length is what is specified bounds - step length is relative to range of x
- bool ignoreBounds

  option to ignore bounds when computing finite diffs
- bool centralHess

option to use old 2nd-order finite diffs for Hessians
- bool warmStartFlag

  if in warm-start mode, don't reset accumulated data (e.g., quasiHessians)
- bool supportsEstimDerivs

  whether model should perform or forward derivative estimation
- String quasiHessType

  quasi-Hessian type: bfgs, damped_bfgs, sr1
- IntSet gradIdAnalytic

  analytic id's for mixed gradients
- IntSet gradIdNumerical

  numerical id's for mixed gradients
- IntSet hessIdAnalytic

  analytic id's for mixed Hessians
- IntSet hessIdNumerical

  numerical id's for mixed Hessians
- IntSet hessIdQuasi

  quasi id's for mixed Hessians
- EvaluationsDBState modelEvaluationsDBState

  Whether to write model evals to the evaluations DB.
- EvaluationsDBState interfEvaluationsDBState

  Whether to write interface evals to the evaluations DB.
- IntArray messageLengths

  length of packed MPI buffers containing vars, vars/set, response, and PRPair
- bool mappingInitialized

  track use of initialize_mapping() and finalize_mapping()
- ProblemDescDB & probDescDB

  class member reference to the problem description database
- ParallelLibrary & parallelLib

  class member reference to the parallel library
- ParConfigLIter modelPCIter

  the ParallelConfiguration node used by this Model instance
- short componentParallelMode

  the component parallelism mode: NO_PARALLEL_MODE, SURROGATE_MODEL_MODE,
- bool asynchEvalFlag

  flags asynch evaluations (local or distributed)
- int evaluationCapacity

  capacity for concurrent evaluations supported by the Model
- short outputLevel

  output verbosity level: {SILENT,QUIET,NORMAL,VERBOSE,DEBUG}_OUTPUT
- Pecos::MultivariateDistribution mvDist

  the multivariate random variable distribution (in probability space corresponding to currentVariables)
- BoolDeque primaryRespFnSense

  array of flags (one per primary function) for switching the sense to maximize the primary function (default is minimize)
- RealVector primaryRespFnWts

  primary response function weightings (either weights for multiobjective optimization or weighted least squares)
- bool hierarchicalTagging

  whether to perform hierarchical evalID tagging of params/results
- ScalingOptions scalingOpts

  user-provided scaling data from the problem DB, possibly modified by Recasting
- String evalTagPrefix

  cached evalTag Prefix from parents to use at evaluate time
- EvaluationStore & evaluationsDB

  reference to the global evaluation database

Private Member Functions

- std::shared_ptr< Model > get_model (ProblemDescDB &problem_db)

    Used by the envelope to instantiate the correct letter class.

- int estimate_derivatives (const ShortArray &map_asv, const ShortArray &fd_grad_asv, const ShortArray &fd-_hess_asv, const ShortArray &quasi_hess_asv, const ActiveSet &original_set, const bool asynch_flag)

    evaluate numerical gradients using finite differences. This routine is selected with "method_source dakota" (the default method_source) in the numerical gradient specification.

- void synchronize_derivatives (const Variables &vars, const IntResponseMap &fd_responses, Response &new_response, const ShortArray &fd_grad_asv, const ShortArray &fd_hess_asv, const ShortArray &quasi-_hess_asv, const ActiveSet &original_set)

    combine results from an array of finite difference response objects (fd_grad_responses) into a single response (new-_response)

- void update_response (const Variables &vars, Response &new_response, const ShortArray &fd_grad_-asv, const ShortArray &fd_hess_asv, const ShortArray &quasi_hess_asv, const ActiveSet &original_set, Response &initial_map_response, const RealMatrix &new_fn_grads, const RealSymMatrixArray &new_fn-_hessians)

    overlay results to update a response object

- void update_quasi_hessians (const Variables &vars, Response &new_response, const ActiveSet &original_-set)

    perform quasi-Newton Hessian updates

- bool manage_asv (const ActiveSet &original_set, ShortArray &map_asv_out, ShortArray &fd_grad_asv_out, ShortArray &fd_hess_asv_out, ShortArray &quasi_hess_asv_out)

    Coordinates usage of estimate_derivatives() calls based on asv_in.

- Real initialize_h (Real x_j, Real lb_j, Real ub_j, Real step_size, String step_type) const

    function to determine initial finite difference h (before step length adjustment) based on type of step desired

- Real FDstep1 (Real x0_j, Real lb_j, Real ub_j, Real h_mag)

    function returning finite-difference step size (affected by bounds)

- Real FDstep2 (Real x0_j, Real lb_j, Real ub_j, Real h)

    function returning second central-difference step size (affected by bounds)

Private Attributes

- int modelEvalCntr

    evaluation counter for top-level evaluate() and evaluate_nowait() calls. Differs from lower level counters in case of numerical derivative estimation (several lower level evaluations are assimilated into a single higher level evaluation)

- bool estDerivsFlag

    flags presence of estimated derivatives within a set of calls to evaluate_nowait()

- bool shortStep

    flags finite-difference step size adjusted by bounds

- std::map< SizetIntPair, ParConfigLIter > modelPCIterMap

    map<> used for tracking modelPCIter instances using depth of parallelism level and max evaluation concurrency as the lookup keys

- bool initCommsBcastFlag

    flag for determining need to bcast the max concurrency from init_communicators(); set from IteratorScheduler::init_-iterator()

- bool modelAutoGraphicsFlag

    flag for posting of graphics data within evaluate() (automatic graphics posting in the model as opposed to graphics posting at the strategy level)

- IntVariablesMap varsMap

    history of vars populated in evaluate_nowait() and used in synchronize().

- std::list< ShortArray > asvList

if estimate_derivatives() is used, transfers ASVs from evaluate_nowait() to synchronize()

- std::list< ActiveSet > setList

  if estimate_derivatives() is used, transfers ActiveSets from evaluate_nowait() to synchronize()

- BoolList initialMapList

  transfers initial_map flag values from estimate_derivatives() to synchronize_derivatives()

- BoolList dbCaptureList

  transfers db_capture flag values from estimate_derivatives() to synchronize_derivatives()

- ResponseList dbResponseList

  transfers database captures from estimate_derivatives() to synchronize_derivatives()

- RealList deltaList

  transfers deltas from estimate_derivatives() to synchronize_derivatives()

- IntIntMap numFDEvalsMap

  tracks the number of evaluations used within estimate_derivatives(). Used in synchronize() as a key for combining finite difference responses into numerical gradients.

- IntIntMap rawEvalIdMap

  maps from the raw evaluation ids returned by derived_synchronize() and derived_synchronize_nowait() to the corresponding modelEvalCntr id. Used for rekeying responseMap.

- RealVectorArray xPrev

  previous parameter vectors used in computing s for quasi-Newton updates

- RealMatrix fnGradsPrev

  previous gradient vectors used in computing y for quasi-Newton updates

- RealSymMatrixArray quasiHessians

  quasi-Newton Hessian approximations

- SizetArray numQuasiUpdates

  number of quasi-Newton Hessian updates applied

- IntResponseMap responseMap

  used to return a map of responses for asynchronous evaluations in final concatenated form. The similar map in Interface contains raw responses.

- IntResponseMap cachedResponseMap

  caching of responses returned by derived_synchronize{,_nowait}() but not matched within current rawEvalIdMap

- IntResponseMap graphicsRespMap

  used to cache the data returned from derived_synchronize_nowait() prior to sequential input into the graphics

- IntSetArray activeDiscSetIntValues

  aggregation of the admissible value sets for all active discrete set integer variables

- StringSetArray activeDiscSetStringValues

  aggregation of the admissible value sets for all active discrete set string variables

- RealSetArray activeDiscSetRealValues

  aggregation of the admissible value sets for all active discrete set real variables

- BitArray discreteIntSets

  key for identifying discrete integer set variables within the active discrete integer variables

- short prevDSIView

  previous view used in discrete_set_int_values(view): avoids recomputation of activeDiscSetIntValues

- short prevDSSView

  previous view used in discrete_set_string_values(view): avoids recomputation of activeDiscSetStringValues

- short prevDSRView

  previous view used in discrete_set_real_values(view): avoids recomputation of activeDiscSetRealValues

- ModelList modelList

  used to collect sub-models for subordinate_models()

- BoolDeque recastFlags

  a key indicating which models within a model recursion involve recasting

- std::shared_ptr< Model > modelRep

  pointer to the letter (initialized only for the envelope)

Static Private Attributes

- static size_t noSpecIdNum = 0

    the last used model ID number for on-the-fly instantiations (increment before each use)

Friends

- bool operator== (const Model &m1, const Model &m2)

    equality operator (detect same letter instance)
- bool operator!= (const Model &m1, const Model &m2)

    inequality operator (detect different letter instances)

14.115.1 Detailed Description

Base class for the model class hierarchy.

The Model class is the base class for one of the primary class hierarchies in DAKOTA. The model hierarchy contains a set of variables, an interface, and a set of responses, and an iterator operates on the model to map the variables into responses using the interface. For memory efficiency and enhanced polymorphism, the model hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Model) serves as the envelope and one of the derived classes (selected in Model::get_model()) serves as the letter.

14.115.2 Constructor & Destructor Documentation

14.115.2.1 Model ( )

default constructor

The default constructor is used in vector<Model> instantiations and for default initialization of Model objects. modelRep is NULL in this case (a populated problem_db is needed to build a meaningful Model object).

14.115.2.2 Model (ProblemDescDB & *problem_db*)

standard constructor for envelope

Used for envelope instantiations within strategy constructors. Envelope constructor only needs to extract enough data to properly execute get_model, since Model(BaseConstructor, problem_db) builds the actual base class data for the derived models.

References Dakota::abort_handler(), and Model::modelRep.

14.115.2.3 Model (const Model & *model*)

copy constructor

Copy constructor manages sharing of modelRep.

14.115.2.4 Model (BaseConstructor , ProblemDescDB & *problem_db*) [protected]

constructor initializing the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor builds the base class data for all inherited models. get_model() instantiates a derived class and the derived class selects this base class constructor in its initialization list (to avoid the recursion of the base class constructor calling get_model() again). Since the letter IS the representation, its representation pointer is set to NULL.

References Dakota::abort_handler(), Model::currentResponse, Dakota::expand_for_fields_sdv(), Model::fdGradStepSize, Model::fdHessByFnStepSize, Model::fdHessByGradStepSize, ProblemDescDB::get_rv(), ProblemDescDB::get_sa(), Model::gradIdNumerical, Model::gradientType, Model::hessianType, Model::hessIdNumerical, Model::initialize_distribution(), Model::initialize_distribution_parameters(), Model::modelId, Model::mvDist, Model::num_primary_fns(), Model::primaryRespFnSense, Model::primaryRespFnWts, Model::probDescDB, Response::shared_data(), Dakota::strbegins(), Dakota::strtolower(), and Model::user_auto_id().

14.115.2.5 Model (LightWtBaseConstructor , ProblemDescDB & *problem_db* = dummy_db, ParallelLibrary & *parallel_lib* = dummy_lib) [protected]

constructor initializing base class for recast model instances

This constructor also builds the base class data for inherited models. However, it is used for derived models which are instantiated on the fly. Therefore it only initializes a small subset of attributes.

14.115.3 Member Function Documentation

14.115.3.1 Iterator & subordinate_iterator ( ) [virtual]

return the sub-iterator in nested and surrogate models

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this operation must be performed on the original envelope object.

Reimplemented in RecastModel, DataFitSurrModel, and NestedModel.

References Dakota::dummy_iterator, and Model::modelRep.

Referenced by NonDExpansion::append_expansion(), NonDMultilevelStochCollocation::assign_specification_sequence(), NonDMultilevelPolynomialChaos::assign_specification_sequence(), SOLBase::check_sub_iterator_conflict(), NonDLocalInterval::check_sub_iterator_conflict(), NonDLocalReliability::check_sub_iterator_conflict(), NCSUOptimizer::check_sub_iterator_conflict(), CONMINOptimizer::check_sub_iterator_conflict(), NonDExpansion::compute_expansion(), SurrBasedGlobalMinimizer::core_run(), NonDExpansion::decrement_grid(), NonDExpansion::decrement_order_and_grid(), NonDExpansion::finalize_sets(), NonDGlobalReliability::get_best_sample(), NonDExpansion::increment_grid(), NonDExpansion::increment_order_and_grid(), NonDExpansion::increment_sets(), NonDMultilevelStochCollocation::increment_specification_sequence(), NonDMultilevelPolynomialChaos::increment_specification_sequence(), NonDExpansion::initialize_expansion(), NonDExpansion::initialize_ml_regression(), NonDExpansion::initialize_u_space_grid(), NonDStochCollocation::initialize_u_space_model(), NonDPolynomialChaos::initialize_u_space_model(), NonDExpansion::merge_grid(), NonDExpansion::pop_increment(), NonDExpansion::pre_refinement(), NonDExpansion::print_refinement_diagnostics(), NonDExpansion::push_increment(), NonDExpansion::select_candidate(), NonDExpansion::select_index_set_candidate(), RecastModel::subordinate_iterator(), NonDExpansion::update_expansion(), NonDBayesCalibration::update_model(), NonDExpansion::update_model_from_samples(), and NonDExpansion::update_u_space_sampler().

14.115.3.2 Model & subordinate_model ( ) [virtual]

return a single sub-model defined from subModel in nested and recast models and truth_model() in surrogate models; used for a directed dive through model recursions that may bypass some components.

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this operation must be performed on the original envelope object.

Reimplemented in RecastModel, NestedModel, and SurrogateModel.

References Dakota::dummy_model, and Model::modelRep.

Referenced by NonDGlobalReliability::expected_feasibility(), NonDGlobalReliability::expected_improvement(), SurrogateModel::force_rebuild(), AdaptedBasisModel::get_sub_model(), Minimizer::initialize_run(), NonDExpansion::initialize_u_space_grid(), NonDGlobalReliability::optimize_gaussian_process(), Minimizer::original_-

model(), COLINOptimizer::post_run(), Optimizer::primary_resp_reducer(), and DataFitSurrModel::update_global_-reference().

14.115.3.3 Model & surrogate_model (size_t *i* = _NPOS) [virtual]

return the active approximation sub-model in surrogate models

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this operation must be performed on the original envelope object.

Reimplemented in RecastModel, DataFitSurrModel, HierarchSurrModel, and NonHierarchSurrModel.

References Dakota::dummy_model, and Model::modelRep.

Referenced by NonDAdaptiveSampling::calc_score_delta_y(), NonDAdaptiveSampling::calc_score_topo_alm_-hybrid(), NonDAdaptiveSampling::calc_score_topo_avg_persistence(), NonDAdaptiveSampling::calc_score_topo-_bottleneck(), NonDMultilevelSampling::configure_indices(), NonDBayesCalibration::construct_mcmc_model(), NonDControlVariateSampling::core_run(), SurrBasedGlobalMinimizer::core_run(), NonDMultilevControlVar-Sampling::evaluate_pilot(), SurrBasedLocalMinimizer::find_approx_response(), NonDControlVariateSampling::hf-_lf_indices(), NonDControlVariateSampling::lf_increment(), NonDMultilevControlVarSampling::multilevel_control_-variate_mc_Qcorr(), NonDAdaptiveSampling::output_round_data(), and RecastModel::surrogate_model().

14.115.3.4 Model & truth_model ( ) [virtual]

return the active truth sub-model in surrogate models

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this operation must be performed on the original envelope object.

Reimplemented in RecastModel, DataFitSurrModel, HierarchSurrModel, and NonHierarchSurrModel.

References Model::modelRep.

Referenced by SurrogateModel::activate_distribution_parameter_derivatives(), NonDMultilevelSampling::compute-_error_estimates(), NonDMultilevelSampling::configure_indices(), NonDControlVariateSampling::core_run(), Surr-BasedGlobalMinimizer::core_run(), SurrogateModel::deactivate_distribution_parameter_derivatives(), NonD-MultilevelSampling::evaluate_ml_sample_increment(), NonDMultilevControlVarSampling::evaluate_pilot(), Surr-BasedLocalMinimizer::find_truth_response(), SurrogateModel::force_rebuild(), NonDControlVariateSampling-::hf_lf_indices(), SurrBasedLocalMinimizer::initialize(), SurrBasedLocalMinimizer::initialize_graphics(), Surr-BasedGlobalMinimizer::initialize_graphics(), NonDC3FunctionTrain::initialize_u_space_model(), NonDMultilevel-FunctionTrain::initialize_u_space_model(), SurrogateModel::insert_response_start(), EnsembleSurrModel-::multifidelity(), EnsembleSurrModel::multilevel(), NonDMultilevControlVarSampling::multilevel_control_variate_mc-_Qcorr(), EnsembleSurrModel::multilevel_multifidelity(), EnsembleSurrModel::nested_acv2_targets(), NonDBayes-Calibration::NonDBayesCalibration(), NonDLocalReliability::NonDLocalReliability(), SurrBasedMinimizer::print_-results(), NonDEnsembleSampling::print_results(), SurrogateModel::probability_transformation(), EnsembleSurr-Model::qoi(), EnsembleSurrModel::query_distribution_parameter_derivatives(), NonDControlVariateSampling-::shared_increment(), EnsembleSurrModel::solution_control_label(), SurrogateModel::subordinate_model(), SurrBasedGlobalMinimizer::SurrBasedGlobalMinimizer(), EnsembleSurrModel::surrogate_response_mode(), SurrogateModel::trans_grad_U_to_X(), SurrogateModel::trans_grad_X_to_S(), SurrogateModel::trans_grad_X-_to_U(), SurrogateModel::trans_hess_X_to_U(), and RecastModel::truth_model().

14.115.3.5 void update_from_subordinate_model (size_t *depth* = SZ_MAX) [virtual]

propagate vars/labels/bounds/targets from the bottom up

used only for instantiate-on-the-fly model recursions (all RecastModel instantiations and alternate DataFitSurrModel instantiations). Simulation, Hierarchical, and Nested Models do not redefine the function since they do not support instantiate-on-the-fly. This means that the recursion will stop as soon as it encounters a Model that was instantiated normally, which is appropriate since ProblemDescDB-constructed Models use top-down information flow and do not require bottom-up updating.

Reimplemented in RecastModel, DataFitSurrModel, HierarchSurrModel, NonHierarchSurrModel, DataTransformModel, and ProbabilityTransformModel.

References Model::modelRep.

Referenced by EffGlobalMinimizer::build_gp(), NonDGlobalInterval::core_run(), NonDLocalInterval::core_run(), NonDExpansion::initialize_expansion(), LeastSq::initialize_run(), Optimizer::initialize_run(), NonDExpansion::multilevel_regression(), NonDGlobalReliability::pre_run(), NonDLocalReliability::pre_run(), NonDBayesCalibration::pre_run(), ProbabilityTransformModel::update_from_subordinate_model(), DataTransformModel::update_from_subordinate_model(), NonHierarchSurrModel::update_from_subordinate_model(), HierarchSurrModel::update_from_subordinate_model(), DataFitSurrModel::update_from_subordinate_model(), and RecastModel::update_from_subordinate_model().

14.115.3.6 Interface & derived_interface ( ) [virtual]

return the interface employed by the derived model class, if present: SimulationModel::userDefinedInterface, DataFitSurrModel::approxInterface, or NestedModel::optionalInterface

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this operation must be performed on the original envelope object.

Reimplemented in RecastModel, DataFitSurrModel, NestedModel, and SimulationModel.

References Dakota::dummy_interface, and Model::modelRep.

Referenced by SurrBasedGlobalMinimizer::core_run(), and RecastModel::derived_interface().

14.115.3.7 size_t solution_levels (bool *lwr_bnd* = true) const [virtual]

number of discrete levels within solution control (SimulationModel)

return the number of levels within a solution / discretization hierarchy.

Reimplemented in SimulationModel.

References Model::modelRep.

Referenced by NonHierarchSurrModel::assign_default_keys(), NonDMultilevelSampling::compute_error_estimates(), NonHierarchSurrModel::create_tabular_datastream(), NonDMultilevControlVarSampling::evaluate_pilot(), EnsembleSurrModel::multifidelity(), EnsembleSurrModel::multilevel(), NonDMultilevControlVarSampling::multilevel_control_variate_mc_Qcorr(), EnsembleSurrModel::multilevel_multifidelity(), HierarchSurrModel::recursive_apply(), and RecastModel::solution_levels().

14.115.3.8 void solution_level_cost_index (size_t *index*) [virtual]

activate a particular level within the solution level control (SimulationModel)

activate a particular level within a solution / discretization hierarchy.

Reimplemented in RecastModel, and SimulationModel.

References Dakota::abort_handler(), and Model::modelRep.

Referenced by NonHierarchSurrModel::assign_default_keys(), NonHierarchSurrModel::assign_key(), NonDMultilevelSampling::configure_indices(), NonDControlVariateSampling::core_run(), NonDControlVariateSampling::hf_lf_indices(), and RecastModel::solution_level_cost_index().

14.115.3.9 short local_eval_synchronization ( ) [virtual]

return derived model synchronization setting

```
SimulationModels and HierarchSurrModels redefine this virtual function.
A default value of "synchronous" prevents asynch local operations for:
```

- NestedModels: a subIterator can support message passing parallelism, but not asynch local.
- DataFitSurrModels: while asynch evals on approximations will work due to some added bookkeeping, avoiding them is preferable.

Reimplemented in RecastModel, SimulationModel, and NestedModel.

References Model::modelRep.

Referenced by Model::init_serial(), RecastModel::local_eval_synchronization(), and Model::set_ie_asynchronous_mode().

14.115.3.10 int local_eval_concurrency ( ) [virtual]

return derived model asynchronous evaluation concurrency

SimulationModels and HierarchSurrModels redefine this virtual function.

Reimplemented in RecastModel, SimulationModel, and NestedModel.

References Model::modelRep.

Referenced by RecastModel::local_eval_concurrency(), and Model::set_ie_asynchronous_mode().

14.115.3.11 const String & interface_id ( ) const [virtual]

return the interface identifier

return by reference requires use of dummy objects, but is important to allow use of assign_rep() since this operation must be performed on the original envelope object.

Reimplemented in RecastModel, DataFitSurrModel, SimulationModel, and NestedModel.

References Dakota::dummy_interface, Interface::interface_id(), and Model::modelRep.

Referenced by NonDDREAMBayesCalibration::archive_acceptance_chain(), Minimizer::archive_best_results(), DataTransformModel::archive_submodel_responses(), DataFitSurrModel::build_global(), NonDMUQBayesCalibration::cache_chain(), NonDQUESOBayesCalibration::cache_chain(), DataFitSurrModel::DataFitSurrModel(), Model::db_lookup(), NonHierarchSurrModel::derived_auto_graphics(), HierarchSurrModel::derived_auto_graphics(), Model::derived_auto_graphics(), Model::estimate_message_lengths(), NonDEnsembleSampling::export_all_samples(), NonDBayesCalibration::export_chain(), NonDBayesCalibration::export_discrepancy(), NonDBayesCalibration::export_field_discrepancy(), SurrBasedLocalMinimizer::find_approx_response(), SurrBasedLocalMinimizer::find_truth_response(), DataFitSurrModel::import_points(), RecastModel::interface_id(), Minimizer::local_recast_retrieve(), NonHierarchSurrModel::matching_all_interface_ids(), HierarchSurrModel::matching_all_interface_ids(), NonHierarchSurrModel::matching_truth_surrogate_interface_ids(), HierarchSurrModel::matching_truth_surrogate_interface_ids(), Analyzer::pre_output(), LeastSq::print_results(), SurrBasedMinimizer::print_results(), Optimizer::print_results(), SeqHybridMetaIterator::run_sequential(), DiscrepancyCorrection::search_db(), Analyzer::update_best(), ConcurrentMetaIterator::update_local_results(), SeqHybridMetaIterator::update_local_results(), and NonDLocalReliability::update_mpp_search_data().

14.115.3.12 bool evaluation_cache (bool *recurse_flag* = true) const [virtual]

Indicates the usage of an evaluation cache by the Model.

Only Models including ApplicationInterfaces support an evaluation cache: surrogate, nested, and recast mappings are not stored in the cache. Possible exceptions: HierarchSurrModel, NestedModel::optionalInterface.

Reimplemented in RecastModel, DataFitSurrModel, HierarchSurrModel, SimulationModel, and NonHierarchSurrModel.

References Model::modelRep.

Referenced by DataFitSurrModel::DataFitSurrModel(), NonHierarchSurrModel::evaluation_cache(), DataFitSurrModel::evaluation_cache(), RecastModel::evaluation_cache(), DataFitSurrModel::import_points(), and Analyzer::read_variables_responses().

14.115.3.13 bool restart_file (bool *recurse_flag* = true) const [virtual]

Indicates the usage of a restart file by the Model.

Only Models including ApplicationInterfaces interact with the restart file: surrogate, nested, and recast mappings are not stored in restart. Possible exceptions: DataFitSurrModel::import_points(), NestedModel::optionalInterface.

Reimplemented in RecastModel, DataFitSurrModel, HierarchSurrModel, SimulationModel, and NonHierarchSurrModel.

References Model::modelRep.

Referenced by DataFitSurrModel::import_points(), Analyzer::read_variables_responses(), NonHierarchSurrModel::restart_file(), DataFitSurrModel::restart_file(), and RecastModel::restart_file().

14.115.3.14 void eval_tag_prefix (const String & *eval_id_str*) [virtual]

set the hierarchical eval ID tag prefix

Derived classes containing additional models or interfaces should implement this function to pass along to their sub Models/Interfaces.

Reimplemented in RecastModel, and SimulationModel.

References Model::evalTagPrefix, and Model::modelRep.

Referenced by HierarchSurrModel::build_approximation(), HierarchSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate(), HierarchSurrModel::derived_evaluate_nowait(), DataFitSurrModel::derived_evaluate_nowait(), Iterator::eval_tag_prefix(), and RecastModel::eval_tag_prefix().

14.115.3.15 ModelList & subordinate_models (bool *recurse_flag* = true)

return the sub-models in nested and surrogate models

since modelList is built with list insertions (using envelope copies), these models may not be used for model.assign_rep() since this operation must be performed on the original envelope object. They may, however, be used for letter-based operations (including assign_rep() on letter contents such as an interface).

References Model::derived_subordinate_models(), Model::modelList, and Model::modelRep.

Referenced by SOLBase::check_sub_iterator_conflict(), NonDLocalInterval::check_sub_iterator_conflict(), NonDLocalReliability::check_sub_iterator_conflict(), NCSUOptimizer::check_sub_iterator_conflict(), CONMINOptimizer::check_sub_iterator_conflict(), NonD::configure_sequence(), NonDMultilevControlVarSampling::core_run(), NonD::inflate_final_samples(), Model::manage_data_recastings(), NonDHierarchSampling::NonDHierarchSampling(), NonDNonHierarchSampling::NonDNonHierarchSampling(), NonD::print_multilevel_evaluation_summary(), and NonD::query_cost().

14.115.3.16 void init_communicators (ParLevLIter *pl_iter,* int *max_eval_concurrency,* bool *recurse_flag* = true)

allocate communicator partitions for a model and store configuration in modelPCIterMap

The init_communicators() and derived_init_communicators() functions are stuctured to avoid performing the messageLengths estimation more than once. init_communicators() (not virtual) performs the estimation and then forwards the results to derived_init_communicators (virtual) which uses the data in different contexts.

References ParallelLibrary::bcast(), Model::derived_init_communicators(), Model::estimate_message_lengths(), ParallelLibrary::increment_parallel_configuration(), Model::initCommsBcastFlag, Model::messageLengths, Model-

::modelPCIter, Model::modelPCIterMap, Model::modelRep, ParallelLibrary::parallel_configuration_iterator(), ParallelLibrary::parallel_level_index(), and Model::parallelLib.

Referenced by AdaptedBasisModel::derived_init_communicators(), NonDGlobalReliability::derived_init_communicators(), NonDLocalInterval::derived_init_communicators(), NonDGlobalInterval::derived_init_communicators(), NonDExpansion::derived_init_communicators(), SurrBasedMinimizer::derived_init_communicators(), NonDAdaptImpSampling::derived_init_communicators(), NonDGPImpSampling::derived_init_communicators(), NonDAdaptiveSampling::derived_init_communicators(), NonDLocalReliability::derived_init_communicators(), ActiveSubspaceModel::derived_init_communicators(), NonDBayesCalibration::derived_init_communicators(), NonDPolynomialChaos::derived_init_communicators(), NonHierarchSurrModel::derived_init_communicators(), HierarchSurrModel::derived_init_communicators(), DataFitSurrModel::derived_init_communicators(), RecastModel::derived_init_communicators(), Iterator::derived_init_communicators(), DataFitSurrModel::derived_set_communicators(), and Model::serve_init_communicators().

14.115.3.17 void init_serial ( )

for cases where init_communicators() will not be called, modify some default settings to behave properly in serial.

The init_serial() and derived_init_serial() functions are stuctured to separate base class (common) operations from derived class (specialized) operations.

References Model::asynchEvalFlag, Model::derived_init_serial(), Model::local_eval_synchronization(), and Model::modelRep.

Referenced by NestedModel::derived_init_serial(), NonHierarchSurrModel::derived_init_serial(), HierarchSurrModel::derived_init_serial(), DataFitSurrModel::derived_init_serial(), and RecastModel::derived_init_serial().

14.115.3.18 void estimate_message_lengths ( )

estimate messageLengths for a model

This functionality has been pulled out of init_communicators() and defined separately so that it may be used in those cases when messageLengths is needed but model.init_communicators() is not called, e.g., for the master processor in the self-scheduling of a concurrent iterator strategy.

References Response::active_set_derivative_vector(), Model::assign_max_strings(), Response::copy(), Variables::copy(), Model::currentResponse, Model::currentVariables, Variables::cv(), Variables::icv(), Model::interface_id(), Model::messageLengths, Model::modelRep, ParallelLibrary::mpirun_flag(), Model::mvDist, Model::numFns, Model::parallelLib, MPIPackBuffer::reset(), and MPIPackBuffer::size().

Referenced by Model::init_communicators(), RandomFieldModel::initialize_mapping(), RecastModel::initialize_mapping(), ConcurrentMetaIterator::pre_run(), Iterator::resize_communicators(), and SubspaceModel::serve_init_mapping().

14.115.3.19 bool manage_data_recastings ( )

initialize modelList and recastFlags for data import/export

Constructor helper to manage model recastings for data import/export.

References Model::modelRep, Model::recastFlags, and Model::subordinate_models().

Referenced by DataFitSurrModel::DataFitSurrModel(), and Analyzer::read_variables_responses().

14.115.3.20 void assign_rep (std::shared_ptr< Model > *model_rep*)

replaces existing letter with a new one

The assign_rep() function is used for publishing derived class letters to existing envelopes, as opposed to sharing representations among multiple envelopes (in particular, assign_rep is passed a letter object and operator= is passed an envelope object).

Use case assumes the incoming letter is instantiated on the fly and has no envelope. This case is modeled after get_model(): a letter is dynamically allocated and passed into assign_rep (its memory management is passed over to the envelope).

If the letter happens to be managed by another envelope, it will persist as long as the last envelope referencing it.

References Model::model_rep(), and Model::modelRep.

Referenced by ActiveSubspaceModel::build_surrogate(), NonDBayesCalibration::calibrate_to_hifi(), ActiveSubspaceModel::compute_cross_validation_metric(), NonDBayesCalibration::construct_map_model(), NonDBayesCalibration::construct_mcmc_model(), DataFitSurrModel::DataFitSurrModel(), ActiveSubspaceModel::get_sub_model(), SurrBasedLocalMinimizer::initialize_sub_model(), EffGlobalMinimizer::initialize_sub_problem(), NonDAdaptImpSampling::NonDAdaptImpSampling(), NonDAdaptiveSampling::NonDAdaptiveSampling(), NonDBayesCalibration::NonDBayesCalibration(), NonDC3FunctionTrain::NonDC3FunctionTrain(), NonDGlobalInterval::NonDGlobalInterval(), NonDGlobalReliability::NonDGlobalReliability(), NonDGPImpSampling::NonDGPImpSampling(), NonDLocalInterval::NonDLocalInterval(), NonDLocalReliability::NonDLocalReliability(), NonDMultilevelFunctionTrain::NonDMultilevelFunctionTrain(), NonDMultilevelPolynomialChaos::NonDMultilevelPolynomialChaos(), NonDMultilevelStochCollocation::NonDMultilevelStochCollocation(), NonDPolynomialChaos::NonDPolynomialChaos(), NonDStochCollocation::NonDStochCollocation(), Optimizer::reduce_model(), NonDPolynomialChaos::resize(), Minimizer::scale_model(), NonDBayesCalibration::scale_model(), LeastSq::weight_model(), and NonDBayesCalibration::weight_model().

14.115.3.21 int derivative_concurrency ( ) const

return the gradient concurrency for use in parallel configuration logic

This function assumes derivatives with respect to the active continuous variables. Therefore, concurrency with respect to the inactive continuous variables is not captured.

References Dakota::contains(), Model::gradIdAnalytic, Model::gradientType, Model::hessianType, Model::hessIdNumerical, Model::intervalType, Model::methodSource, Model::modelRep, and Model::numDerivVars.

Referenced by ActiveSubspaceModel::ActiveSubspaceModel(), NonHierarchSurrModel::derived_free_communicators(), HierarchSurrModel::derived_free_communicators(), NonHierarchSurrModel::derived_init_communicators(), HierarchSurrModel::derived_init_communicators(), DataFitSurrModel::derived_init_communicators(), HierarchSurrModel::derived_set_communicators(), DataFitSurrModel::estimate_partition_bounds(), NonDExpansion::initialize_u_space_grid(), Analyzer::num_samples(), HierarchSurrModel::serve_run(), and Iterator::update_from_model().

14.115.3.22 void active_variables (const RealVector & *config_vars*, Model & *model*) [static]

set the specified configuration to the Model's inactive vars, converting from real to integer or through index to string value as needed

config_vars consists of [continuous, integer, string, real].

References Model::continuous_variables(), Model::current_variables(), Model::cv(), Model::discrete_int_variables(), Model::discrete_real_variables(), Model::discrete_set_string_values(), Variables::discrete_string_variable(), Model::div(), Model::drv(), Model::dsv(), Dakota::iround(), and Dakota::set_index_to_value().

14.115.3.23 void inactive_variables (const RealVector & *config_vars*, Model & *model*) [static]

set the specified configuration to the Model's inactive vars, converting from real to integer or through index to string value as needed

config_vars consists of [continuous, integer, string, real].

References Model::current_variables(), and Model::inactive_variables().

14.115.3.24 void inactive_variables (const RealVector & *config_vars*, Model & *model*, Variables & *vars*) [static]

config_vars consists of [continuous, integer, string, real].

References Model::current_variables(), Model::discrete_set_string_values(), Model::icv(), Model::idiv(), Model::idrv(), Model::idsv(), Variables::inactive_continuous_variables(), Variables::inactive_discrete_int_variables(), Variables::inactive_discrete_real_variables(), Variables::inactive_discrete_string_variable(), Dakota::iround(), Dakota::set_index_to_value(), and Variables::view().

14.115.3.25 String user_auto_id ( ) [static], [protected]

return the next available model ID for no-ID user methods

Rationale: The parser allows multiple user-specified models with empty (unspecified) ID. However, only a single Model with empty ID can be constructed (if it's the only one present, or the "last one parsed"). Therefore decided to prefer NO_MODEL_ID over NO_MODEL_ID_<num> for (some) consistency with interface NO_ID convention. *MODEL* was inserted in the middle to distinguish "anonymous" MODELS from methods and interfaces in the hdf5 output. Note that this function is not used to name recast models; see their constructors for how its done.

Referenced by Model::Model().

14.115.3.26 String no_spec_id ( ) [static], [protected]

return the next available model ID for on-the-fly methods

Rationale: For now NOSPEC_MODEL_ID_ is chosen due to historical id="NO_SPECIFICATION" used for internally-constructed Models. Longer-term, consider auto-generating an ID that includes the context from which the method is constructed, e.g., the parent method or model's ID, together with its name. Note that this function is not used to name recast models; see their constructors for how its done.

References Model::noSpecIdNum.

14.115.3.27 void initialize_distribution (Pecos::MultivariateDistribution & *mv_dist,* bool *active_only* = false) [protected]

initialize distribution types from problemDescDB

Build random variable distribution types and active subset. This function is used when the Model variables are in x-space.

References SharedVariablesData::active_subsets(), Dakota::assign_value(), Model::currentVariables, Variables::cv(), Variables::div(), Variables::drv(), Variables::dsv(), Model::dsv(), ProblemDescDB::get_rv(), ProblemDescDB::get_sizet(), Model::probDescDB, Variables::shared_data(), and Variables::tv().

Referenced by Model::Model().

14.115.3.28 std::shared_ptr< Model > get_model (ProblemDescDB & *problem_db*) [private]

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize modelRep to the appropriate derived type, as given by the modelType attribute.

References ProblemDescDB::get_string(), and Model::model_type().

14.115.3.29 int estimate_derivatives (const ShortArray & *map_asv,* const ShortArray & *fd_grad_asv,* const ShortArray & *fd_hess_asv,* const ShortArray & *quasi_hess_asv,* const ActiveSet & *original_set,* const bool *asynch_flag*) [private]

evaluate numerical gradients using finite differences. This routine is selected with "method_source dakota" (the default method_source) in the numerical gradient specification.

Estimate derivatives by computing finite difference gradients, finite difference Hessians, and/or quasi-Newton Hessians. The total number of finite difference evaluations is returned for use by synchronize() to track response arrays, and it could be used to improve management of max_function_evaluations within the iterators. ! new logic

References Variables::all_continuous_variables(), Model::centralHess, Variables::continuous_variables(), Model::currentResponse, Model::currentVariables, Model::db_lookup(), Model::dbCaptureList, Model::dbResponseList, Model::deltaList, ActiveSet::derivative_vector(), Model::derived_evaluate(), Model::derived_evaluate_nowait(), Model::fdHessByFnStepSize, Model::fdHessByGradStepSize, Model::fdHessStepType, Model::FDstep1(), Model::FDstep2(), Dakota::find_index(), Model::forward_grad_step(), Response::function_gradients(), Response::function_values(), Model::ignoreBounds, Variables::inactive_continuous_variables(), Model::initialize_h(), Model::initialize_x0_bounds(), Model::initialMapList, Model::intervalType, Model::numFns, Model::outputLevel, ActiveSet::request_vector(), Response::shared_data(), Model::shortStep, and Model::update_response().

Referenced by Model::evaluate(), and Model::evaluate_nowait().

14.115.3.30 void synchronize_derivatives (const **Variables** & *vars,* const IntResponseMap & *fd_responses,* **Response** & *new_response,* const ShortArray & *fd_grad_asv,* const ShortArray & *fd_hess_asv,* const ShortArray & *quasi_hess_asv,* const **ActiveSet** & *original_set*) [private]

combine results from an array of finite difference response objects (fd_grad_responses) into a single response (new_response)

Merge an array of fd_responses into a single new_response. This function is used both by synchronous evaluate() for the case of asynchronous estimate_derivatives() and by synchronize() for the case where one or more evaluate_nowait() calls has employed asynchronous estimate_derivatives(). !

References Model::acv(), Variables::all_continuous_variable_ids(), Model::centralHess, Variables::continuous_variable_ids(), Model::currentResponse, Model::currentVariables, Model::cv(), Model::dbCaptureList, Model::dbResponseList, Model::deltaList, ActiveSet::derivative_vector(), Dakota::find_index(), Response::function_gradients(), Response::function_values(), Model::icv(), Variables::inactive_continuous_variable_ids(), Model::initialMapList, Model::intervalType, Model::numFns, Response::shared_data(), and Model::update_response().

Referenced by Model::evaluate(), and Model::synchronize().

14.115.3.31 void update_response (const **Variables** & *vars,* **Response** & *new_response,* const ShortArray & *fd_grad_asv,* const ShortArray & *fd_hess_asv,* const ShortArray & *quasi_hess_asv,* const **ActiveSet** & *original_set,* **Response** & *initial_map_response,* const RealMatrix & *new_fn_grads,* const RealSymMatrixArray & *new_fn_hessians*) [private]

overlay results to update a response object

Overlay the initial_map_response with numerically estimated new_fn_grads and new_fn_hessians to populate new_response as governed by asv vectors. Quasi-Newton secant Hessian updates are also performed here, since this is where the gradient data needed for the updates is first consolidated. Convenience function used by estimate_derivatives() for the synchronous case and by synchronize_derivatives() for the asynchronous case.

References Response::active_set_request_vector(), Variables::continuous_variable_ids(), Response::copy(), Model::currentResponse, Model::currentVariables, ActiveSet::derivative_vector(), Response::function_gradients(), Response::function_hessians(), Response::function_values(), Model::hessianType, Model::hessIdQuasi, Response::is_null(), Model::numFns, Model::outputLevel, Model::quasiHessians, ActiveSet::request_vector(), Response::reset_inactive(), Model::supportsEstimDerivs, Model::surrogate_response_mode(), and Model::update_quasi_hessians().

Referenced by Model::estimate_derivatives(), and Model::synchronize_derivatives().

14.115.3.32 void update_quasi_hessians (const **Variables** & *vars,* **Response** & *new_response,* const **ActiveSet** & *original_set*) [private]

perform quasi-Newton Hessian updates

quasi-Newton updates are performed for approximating response function Hessians using BFGS or SR1 formulations. These Hessians are supported only for the active continuous variables, and a check is performed on the DVV prior to invoking the function.

References Dakota::contains(), Variables::continuous_variables(), Dakota::copy_data(), Model::fnGradsPrev, Response::function_gradients(), Model::hessianType, Model::hessIdQuasi, Model::modelType, Model::numDerivVars, Model::numFns, Model::numQuasiUpdates, Model::outputLevel, Model::quasiHessians, Model::quasiHessType, ActiveSet::request_vector(), and Model::xPrev.

Referenced by Model::update_response().

14.115.3.33 bool manage_asv (const ActiveSet & *original_set,* ShortArray & *map_asv_out,* ShortArray & *fd_grad_asv_out,* ShortArray & *fd_hess_asv_out,* ShortArray & *quasi_hess_asv_out*) [private]

Coordinates usage of estimate_derivatives() calls based on asv_in.

Splits asv_in total request into map_asv_out, fd_grad_asv_out, fd_hess_asv_out, and quasi_hess_asv_out as governed by the responses specification. If the returned use_est_deriv is true, then these asv outputs are used by estimate_derivatives() for the initial map, finite difference gradient evals, finite difference Hessian evals, and quasi--Hessian updates, respectively. If the returned use_est_deriv is false, then only map_asv_out is used.

References Dakota::abort_handler(), Dakota::contains(), ActiveSet::derivative_vector(), Model::FDstep2(), Dakota::find_index(), Model::forward_grad_step(), Model::gradIdAnalytic, Model::gradIdNumerical, Model::gradientType, Model::hessianType, Model::hessIdAnalytic, Model::hessIdNumerical, Model::hessIdQuasi, Model::ignoreBounds, Model::initialize_x0_bounds(), Model::intervalType, Model::methodSource, Model::model_id(), ActiveSet::request_vector(), Model::shortStep, Model::supportsEstimDerivs, and Model::surrogate_response_mode().

Referenced by Model::evaluate(), and Model::evaluate_nowait().

14.115.3.34 Real initialize_h (Real *x_j,* Real *lb_j,* Real *ub_j,* Real *step_size,* String *step_type*) const [private]

function to determine initial finite difference h (before step length adjustment) based on type of step desired

Auxiliary function to determine initial finite difference h (before step length adjustment) based on type of step desired.

Referenced by Model::estimate_derivatives(), and Model::forward_grad_step().

14.115.3.35 Real FDstep1 (Real *x0_j,* Real *lb_j,* Real *ub_j,* Real *h_mag*) [private]

function returning finite-difference step size (affected by bounds)

Auxiliary function to compute forward or first central-difference step size, honoring bounds. The first step is away from zero, when possible. Flips the direction or updates shortStep if can't take the full requested step h_mag.

References Model::ignoreBounds, and Model::shortStep.

Referenced by Model::estimate_derivatives(), and Model::forward_grad_step().

14.115.3.36 Real FDstep2 (Real *x0_j,* Real *lb_j,* Real *ub_j,* Real *h*) [private]

function returning second central-difference step size (affected by bounds)

Auxiliary function to compute the second central-difference step size, honoring bounds.

References Model::ignoreBounds, and Model::shortStep.

Referenced by Model::estimate_derivatives(), and Model::manage_asv().

14.115.4 Member Data Documentation

14.115.4.1 RealVector fdGradStepSize [protected]

relative finite difference step size for numerical gradients

A scalar value (instead of the vector fd_gradient_step_size spec) is used within the iterator hierarchy since this attribute is only used to publish a step size to vendor numerical gradient algorithms.

Referenced by DataFitSurrModel::DataFitSurrModel(), Model::fd_gradient_step_size(), Model::forward_grad_-step(), RecastModel::initialize_data_from_submodel(), and Model::Model().

14.115.4.2 RealVector fdHessByGradStepSize [protected]

relative finite difference step size for numerical Hessians estimated using first-order differences of gradients

For vendor numerical Hessian algorithms, a scalar value is used.

Referenced by DataFitSurrModel::DataFitSurrModel(), Model::estimate_derivatives(), Model::fd_hessian_by_grad-_step_size(), RecastModel::initialize_data_from_submodel(), and Model::Model().

14.115.4.3 RealVector fdHessByFnStepSize [protected]

relative finite difference step size for numerical Hessians estimated using second-order differences of function values

For vendor numerical Hessian algorithms, a scalar value is used.

Referenced by DataFitSurrModel::DataFitSurrModel(), Model::estimate_derivatives(), Model::fd_hessian_by_fn_-step_size(), RecastModel::initialize_data_from_submodel(), and Model::Model().

14.115.4.4 ProblemDescDB& probDescDB [protected]

class member reference to the problem description database

Iterator and Model cannot use a shallow copy of ProblemDescDB due to circular destruction dependency (reference counts can't get to 0), since ProblemDescDB contains {iterator,model}List.

Referenced by ActiveSubspaceModel::ActiveSubspaceModel(), NestedModel::derived_init_communicators(), Non-HierarchSurrModel::derived_init_communicators(), HierarchSurrModel::derived_init_communicators(), DataFit-SurrModel::derived_init_communicators(), NestedModel::derived_init_serial(), NestedModel::estimate_partition-_bounds(), SimulationModel::estimate_partition_bounds(), NonHierarchSurrModel::estimate_partition_bounds(), HierarchSurrModel::estimate_partition_bounds(), DataFitSurrModel::estimate_partition_bounds(), NestedModel-::init_sub_iterator(), Model::initialize_distribution(), Model::initialize_distribution_parameters(), Model::Model(), Model::problem_description_db(), and SimulationModel::SimulationModel().

The documentation for this class was generated from the following files:

- DakotaModel.hpp
- DakotaModel.cpp

14.116 MPIManager Class Reference

Class MPIManager to manage Dakota's MPI world, which may be a subset of MPI_COMM_WORLD.

Public Member Functions

- MPIManager ()

    Default constructor; Dakota will not call MPI_Init.
- MPIManager (int &argc, char **&argv)

Command-line constructor; parses MPI arguments during call to MPI_Init.

- MPIManager (MPI_Comm dakota_mpi_comm)

    Construct on specified MPI_Comm.

- ∼MPIManager ()

    destructor: calls finalize if Dakota owns MPI

- MPI_Comm dakota_mpi_comm () const

    get the MPI_Comm on which Dakota is running

- int world_rank () const

    get the rank of this process in Dakota's MPI_Comm

- int world_size () const

    get the size of the MPI_Comm on which Dakota is running

- bool mpirun_flag () const

    true when Dakota is running in MPI mode

Static Public Member Functions

- static bool detect_parallel_launch (int &argc, char ∗∗&argv)

    detect parallel launch of Dakota using mpirun/mpiexec/poe/etc. based on command line arguments and environment variables

Private Attributes

- MPI_Comm dakotaMPIComm

    MPI_Comm on which DAKOTA is running.

- int dakotaWorldRank

    rank in MPI_Comm in which DAKOTA is running

- int dakotaWorldSize

    size of MPI_Comm in which DAKOTA is running

- bool mpirunFlag

    flag for a parallel mpirun/yod launch

- bool ownMPIFlag

    flag for ownership of MPI_Init/MPI_Finalize

14.116.1 Detailed Description

Class MPIManager to manage Dakota's MPI world, which may be a subset of MPI_COMM_WORLD.

The documentation for this class was generated from the following files:

- MPIManager.hpp
- MPIManager.cpp

14.117 MPIPackBuffer Class Reference

Class for packing MPI message buffers.

Public Member Functions

- MPIPackBuffer (int size_=1024)

  Constructor, which allows the default buffer size to be set.
- ∼MPIPackBuffer ()

  Desctructor.
- const char ∗ buf ()

  Returns a pointer to the internal buffer that has been packed.
- int size ()

  The number of bytes of packed data.
- int capacity ()

  the allocated size of Buffer.
- void reset ()

  Resets the buffer index in order to reuse the internal buffer.
- void pack (const int ∗data, const int num=1)

  *Pack one or more **int's**.*
- void pack (const u_int ∗data, const int num=1)

  *Pack one or more **unsigned int's**.*
- void pack (const long ∗data, const int num=1)

  *Pack one or more **long's**.*
- void pack (const u_long ∗data, const int num=1)

  *Pack one or more **unsigned long's**.*
- void pack (const long long ∗data, const int num=1)

  Pack one or more long long's.
- void pack (const unsigned long long ∗data, const int num=1)

  Pack one or more unsigned long long's.
- void pack (const short ∗data, const int num=1)

  *Pack one or more **short's**.*
- void pack (const u_short ∗data, const int num=1)

  *Pack one or more **unsigned short's**.*
- void pack (const char ∗data, const int num=1)

  *Pack one or more **char's**.*
- void pack (const u_char ∗data, const int num=1)

  *Pack one or more **unsigned char's**.*
- void pack (const double ∗data, const int num=1)

  *Pack one or more **double's**.*
- void pack (const float ∗data, const int num=1)

  *Pack one or more **float's**.*
- void pack (const bool ∗data, const int num=1)

  *Pack one or more **bool's**.*
- void pack (const int &data)

  *Pack a **int**.*
- void pack (const u_int &data)

  *Pack a **unsigned int**.*
- void pack (const long &data)

  *Pack a **long**.*
- void pack (const u_long &data)

  *Pack a **unsigned long**.*
- void pack (const long long &data)

  Pack a long long.
- void pack (const unsigned long long &data)

Pack a unsigned long long.
- void pack (const short &data)

    *Pack a **short**.*
- void pack (const u_short &data)

    *Pack a **unsigned short**.*
- void pack (const char &data)

    *Pack a **char**.*
- void pack (const u_char &data)

    *Pack a **unsigned char**.*
- void pack (const double &data)

    *Pack a **double**.*
- void pack (const float &data)

    *Pack a **float**.*
- void pack (const bool &data)

    *Pack a **bool**.*

Protected Member Functions

- void resize (const int newsize)

    Resizes the internal buffer.

Protected Attributes

- char ∗ Buffer

    The internal buffer for packing.
- int Index

    The index into the current buffer.
- int Size

    The total size that has been allocated for the buffer.

14.117.1 Detailed Description

Class for packing MPI message buffers.

A class that provides a facility for packing message buffers using the MPI_Pack facility. The `MPIPackBuffer` class dynamically resizes the internal buffer to contain enough memory to pack the entire object. When deleted, the `MPIPackBuffer` object deletes this internal buffer. This class is based on the Dakota_Version_3_0 version of utilib::PackBuffer from utilib/src/io/PackBuf.[cpp,h]. This snapshot preceded the introduction of templatization on data type, which was problematic at that time (would be more reliable now).

The documentation for this class was generated from the following files:

- MPIPackBuffer.hpp
- MPIPackBuffer.cpp

14.118 MPIUnpackBuffer Class Reference

Class for unpacking MPI message buffers.

Public Member Functions

- void setup (char *buf_, int size_, bool flag_=false)

  Method that does the setup for the constructors.
- MPIUnpackBuffer ()

  Default constructor.
- MPIUnpackBuffer (int size_)

  Constructor that specifies the size of the buffer.
- MPIUnpackBuffer (char *buf_, int size_, bool flag_=false)

  Constructor that sets the internal buffer to the given array.
- ∼MPIUnpackBuffer ()

  Destructor.
- void resize (const int newsize)

  Resizes the internal buffer.
- const char * buf ()

  Returns a pointer to the internal buffer.
- int size ()

  Returns the length of the buffer.
- int curr ()

  Returns the number of bytes that have been unpacked from the buffer.
- void reset ()

  Resets the index of the internal buffer.
- void unpack (int *data, const int num=1)

  *Unpack one or more **int's**.*
- void unpack (u_int *data, const int num=1)

  *Unpack one or more **unsigned int's**.*
- void unpack (long *data, const int num=1)

  *Unpack one or more **long's**.*
- void unpack (u_long *data, const int num=1)

  *Unpack one or more **unsigned long's**.*
- void unpack (long long *data, const int num=1)

  Unpack one or more long long's.
- void unpack (unsigned long long *data, const int num=1)

  Unpack one or more unsigned long long's.
- void unpack (short *data, const int num=1)

  *Unpack one or more **short's**.*
- void unpack (u_short *data, const int num=1)

  *Unpack one or more **unsigned short's**.*
- void unpack (char *data, const int num=1)

  *Unpack one or more **char's**.*
- void unpack (u_char *data, const int num=1)

  *Unpack one or more **unsigned char's**.*
- void unpack (double *data, const int num=1)

  *Unpack one or more **double's**.*
- void unpack (float *data, const int num=1)

  *Unpack one or more **float's**.*
- void unpack (bool *data, const int num=1)

  *Unpack one or more **bool's**.*
- void unpack (int &data)

  *Unpack a **int**.*
- void unpack (u_int &data)

*Unpack a **unsigned int**.*

- void unpack (long &data)

    *Unpack a **long**.*

- void unpack (u_long &data)

    *Unpack a **unsigned long**.*

- void unpack (long long &data)

    Unpack a long long.

- void unpack (unsigned long long &data)

    Unpack a unsigned long long.

- void unpack (short &data)

    *Unpack a **short**.*

- void unpack (u_short &data)

    *Unpack a **unsigned short**.*

- void unpack (char &data)

    *Unpack a **char**.*

- void unpack (u_char &data)

    *Unpack a **unsigned char**.*

- void unpack (double &data)

    *Unpack a **double**.*

- void unpack (float &data)

    *Unpack a **float**.*

- void unpack (bool &data)

    *Unpack a **bool**.*

Protected Attributes

- char ∗ Buffer

    The internal buffer for unpacking.

- int Index

    The index into the current buffer.

- int Size

    The total size that has been allocated for the buffer.

- bool ownFlag

    If `TRUE`, then this class owns the internal buffer.

14.118.1 Detailed Description

Class for unpacking MPI message buffers.

A class that provides a facility for unpacking message buffers using the MPI_Unpack facility. This class is based on the Dakota_Version_3_0 version of utilib::UnPackBuffer from utilib/src/io/PackBuf.[cpp,h]

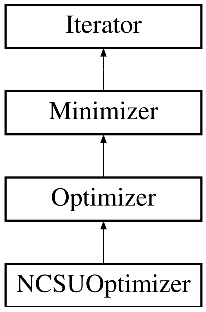
The documentation for this class was generated from the following files:

- MPIPackBuffer.hpp
- MPIPackBuffer.cpp

14.119 NCSUOptimizer Class Reference

Wrapper class for the NCSU DIRECT optimization library.

Inheritance diagram for NCSUOptimizer:



Public Member Functions

- NCSUOptimizer (ProblemDescDB &problem_db, Model &model)

    standard constructor
- NCSUOptimizer (Model &model, size_t max_iter, size_t max_eval, double min_box_size=-1., double vol_box_size=-1., double solution_target=-DBL_MAX)

    alternate constructor for instantiations "on the fly"
- NCSUOptimizer (Model &model)

    alternate constructor for Iterator instantiations by name
- NCSUOptimizer (const RealVector &var_l_bnds, const RealVector &var_u_bnds, size_t max_iter, size_t max_eval, double(∗user_obj_eval)(const RealVector &x), double min_box_size=-1., double vol_box_size=-1., double solution_target=-DBL_MAX)

    alternate constructor for instantiations "on the fly"
- ∼NCSUOptimizer ()

    destructor
- void core_run ()

    core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void declare_sources ()

    Declare sources to the evaluations database.
- void check_sub_iterator_conflict ()

    detect any conflicts due to recursive use of the same Fortran solver

Private Member Functions

- void initialize ()

    shared code among model-based constructors
- void check_inputs ()

    verify problem respects NCSU DIRECT Fortran limits

Static Private Member Functions

- static int objective_eval (int ∗n, double c[ ], double l[ ], double u[ ], int point[ ], int ∗maxI, int ∗start, int ∗maxfunc, double fvec[ ], int iidata[ ], int ∗iisize, double ddata[ ], int ∗idsize, char cdata[ ], int ∗icsize)

    'fep' in Griffin-modified NCSUDirect: computes the value of the objective function (potentially at multiple points, passed by function pointer to NCSUDirect). Include unscaling from DIRECT.

Private Attributes

- short setUpType

  controls iteration mode: SETUP_MODEL (normal usage) or SETUP_USERFUNC (user-supplied functions mode for "on the fly" instantiations). see enum in NCSUOptimizer.cpp NonDGlobalReliability currently uses the model mode. GaussProcApproximation currently uses the user_functions mode.
- Real minBoxSize

  holds the minimum boxsize
- Real volBoxSize

  hold the minimum volume boxsize
- Real solutionTarget

  holds the solution target minimum to drive towards
- RealVector lowerBounds

  holds variable lower bounds passed in for "user_functions" mode.
- RealVector upperBounds

  holds variable upper bounds passed in for "user_functions" mode.
- double(∗ userObjectiveEval)(const RealVector &x)

  holds function pointer for objective function evaluator passed in for "user_functions" mode.

Static Private Attributes

- static NCSUOptimizer ∗ ncsudirectInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

14.119.1 Detailed Description

Wrapper class for the NCSU DIRECT optimization library.

The NCSUOptimizer class provides a wrapper for a Fortran 77 implementation of the DIRECT algorithm developed at North Carolina State University. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any attribute used within static member functions must be either local to that function or accessed through a static pointer.

The user input mappings are as follows:

14.119.2 Constructor & Destructor Documentation

14.119.2.1 NCSUOptimizer (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This is the standard constructor with method specification support.

References NCSUOptimizer::check_inputs().

14.119.2.2 NCSUOptimizer (Model & *model,* size_t *max_iter,* size_t *max_eval,* double *min_box_size* = `-1.`, double *vol_box_size* = `-1.`, double *solution_target* = `-DBL_MAX`)

alternate constructor for instantiations "on the fly"

This is an alternate constructor for instantiations on the fly using a Model but no ProblemDescDB.

References NCSUOptimizer::check_inputs(), Iterator::maxFunctionEvals, and Iterator::maxIterations.

14.119.2.3 NCSUOptimizer (Model & *model*)

alternate constructor for Iterator instantiations by name

This is an alternate constructor for Iterator instantiations by name using a Model but no ProblemDescDB.

References NCSUOptimizer::check_inputs().

14.119.2.4 NCSUOptimizer (const RealVector & *var_l_bnds,* const RealVector & *var_u_bnds,* size_t *max_iter,* size_t *max_eval,* double(∗)(const RealVector &x) *user_obj_eval,* double *min_box_size =* `-1.`, double *vol_box_size =* `-1.`, double *solution_target =* `-DBL_MAX`)

alternate constructor for instantiations "on the fly"

This is an alternate constructor for performing an optimization using the passed in objective function pointer.

References NCSUOptimizer::check_inputs(), Iterator::maxFunctionEvals, and Iterator::maxIterations.

14.119.3 Member Function Documentation

14.119.3.1 void core_run ( ) `[virtual]`

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Dakota::abort_handler(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Model::continuous-_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Iterator::convergenceTol, Dakota::copy_data(), Iterator::iteratedModel, Optimizer::localObjectiveRecast, NCSUOptimizer::lowerBounds, Iterator::maxFunctionEvals, Iterator::maxIterations, NCSUOptimizer::minBoxSize, NCSUOptimizer::ncsudirect-Instance, Minimizer::numContinuousVars, Minimizer::numFunctions, NCSUOptimizer::objective_eval(), Iterator-::outputLevel, Model::primary_response_fn_sense(), NCSUOptimizer::setUpType, NCSUOptimizer::solutionTarget, NCSUOptimizer::upperBounds, and NCSUOptimizer::volBoxSize.

14.119.3.2 void check_sub_iterator_conflict ( ) `[virtual]`

detect any conflicts due to recursive use of the same Fortran solver

This is used to avoid clashes in state between non-object-oriented (i.e., F77, C) iterator executions, when such iterators could potentially be executing simultaneously (e.g., nested execution). It is not an issue (and a used method is not reported) in cases where a helper execution is completed before a lower level one could be initiated; an example of this is DIRECT for maximization of expected improvement: the EIF maximization is completed before a new point evaluation (which could include nested iteration) is performed.

Reimplemented from Iterator.

References Iterator::is_null(), Iterator::iteratedModel, Iterator::method_name(), Iterator::method_recourse(), Model-::subordinate_iterator(), Model::subordinate_models(), and Iterator::uses_method().

14.119.3.3 int objective_eval (int ∗ *n,* double *c[ ],* double *l[ ],* double *u[ ],* int *point[ ],* int ∗ *maxI,* int ∗ *start,* int ∗ *maxfunc,* double *fvec[ ],* int *iidata[ ],* int ∗ *iisize,* double *ddata[ ],* int ∗ *idsize,* char *cdata[ ],* int ∗ *icsize*) `[static]`, `[private]`

'fep' in Griffin-modified NCSUDirect: computes the value of the objective function (potentially at multiple points, passed by function pointer to NCSUDirect). Include unscaling from DIRECT.

Modified batch evaluator that accepts multiple points and returns corresponding vector of functions in fvec. Must be used with modified DIRECT src (DIRbatch.f).

References Model::asynch_flag(), Model::continuous_variables(), Model::current_response(), Model::evaluate(), Model::evaluate_nowait(), Response::function_value(), Iterator::iteratedModel, NCSUOptimizer::ncsudirectInstance, Model::primary_response_fn_sense(), NCSUOptimizer::setUpType, Model::synchronize(), and NCSUOptimizer::userObjectiveEval.

Referenced by NCSUOptimizer::core_run().

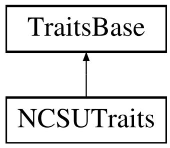
The documentation for this class was generated from the following files:

- NCSUOptimizer.hpp
- NCSUOptimizer.cpp

14.120 NCSUTraits Class Reference

A version of TraitsBase specialized for NCSU optimizers.

Inheritance diagram for NCSUTraits:



Public Member Functions

- NCSUTraits ()
  default constructor
- virtual ∼NCSUTraits ()
  destructor
- virtual bool is_derived ()
  A temporary query used in the refactor.
- bool supports_continuous_variables ()
  Return the flag indicating whether method supports continuous variables.

14.120.1 Detailed Description

A version of TraitsBase specialized for NCSU optimizers.

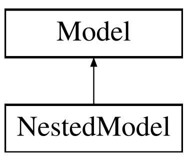
The documentation for this class was generated from the following file:

- NCSUOptimizer.hpp

14.121 NestedModel Class Reference

Derived model class which performs a complete sub-iterator execution within every evaluation of the model.

Inheritance diagram for NestedModel:



Public Member Functions

- NestedModel (ProblemDescDB &problem_db)

  constructor
- ∼NestedModel ()

  destructor
- void declare_sources ()

  Declare a model's sources to the evaluationsDB.

Protected Member Functions

- void derived_evaluate (const ActiveSet &set)

  portion of evaluate() specific to NestedModel
- void derived_evaluate_nowait (const ActiveSet &set)

  portion of evaluate_nowait() specific to NestedModel
- const IntResponseMap & derived_synchronize ()

  portion of synchronize() specific to NestedModel
- Iterator & subordinate_iterator ()

  return subIterator
- Model & subordinate_model ()

  return subModel
- void derived_subordinate_models (ModelList &ml, bool recurse_flag)

  return subModel
- Interface & derived_interface ()

  return optionalInterface
- const RealVector & error_estimates ()

  retrieve error estimates corresponding to the subIterator's response results (e.g., statistical MSE for subordinate UQ).
- void surrogate_response_mode (short mode)

  pass a bypass request on to the subModel for any lower-level surrogates
- void component_parallel_mode (short mode)

  update component parallel mode for supporting parallelism in optionalInterface and subModel
- size_t mi_parallel_level_index () const

  return subIteratorSched.miPLIndex
- short local_eval_synchronization ()

  return optionalInterface synchronization setting
- int local_eval_concurrency ()

  return optionalInterface asynchronous evaluation concurrency
- bool derived_master_overload () const

  flag which prevents overloading the master with a multiprocessor evaluation (forwarded to optionalInterface)
- IntIntPair estimate_partition_bounds (int max_eval_concurrency)

  estimate the minimum and maximum partition sizes that can be utilized by this Model
- void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set up optionalInterface and subModel for parallel operations
- void derived_init_serial ()

  set up optionalInterface and subModel for serial operations.
- void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set active parallel configuration within subModel
- void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  deallocate communicator partitions for the NestedModel (forwarded to optionalInterface and subModel)
- void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)

Service optionalInterface and subModel job requests received from the master. Completes when a termination message is received from stop_servers().

- void stop_servers ()

  Executed by the master to terminate server operations for subModel and optionalInterface when iteration on the NestedModel is complete.

- const String & interface_id () const

  return the optionalInterface identifier

- int derived_evaluation_id () const

  Return the current evaluation id for the NestedModel.

- void set_evaluation_reference ()

  set the evaluation counter reference points for the NestedModel (request forwarded to optionalInterface and subModel)

- void fine_grained_evaluation_counters ()

  request fine-grained evaluation reporting within optionalInterface and subModel

- void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const

  print the evaluation summary for the NestedModel (request forwarded to optionalInterface and subModel)

- void warm_start_flag (const bool flag)

  set the warm start flag, including actualModel

- void **initialize_iterator** (int job_index)
- void **pack_parameters_buffer** (MPIPackBuffer &send_buffer, int job_index)
- void **unpack_parameters_buffer** (MPIUnpackBuffer &recv_buffer, int job_index)
- void **unpack_parameters_initialize** (MPIUnpackBuffer &recv_buffer, int job_index)
- void **pack_results_buffer** (MPIPackBuffer &send_buffer, int job_index)
- void **unpack_results_buffer** (MPIUnpackBuffer &recv_buffer, int job_index)
- void **update_local_results** (int job_index)
- ActiveSet **default_interface_active_set** ()

Private Member Functions

- void init_sub_iterator ()

  init subIterator-based counts and init subModel with mapping data

- PRPQueueIter job_index_to_queue_iterator (int job_index)

  convert job_index to an eval_id through subIteratorIdMap and eval_id to a subIteratorPRPQueue queue iterator

- void initialize_iterator (const Variables &vars, const ActiveSet &set, int eval_id)

  lower level function shared by initialize_iterator(int) and unpack_parameters_initialize()

- void unpack (MPIUnpackBuffer &recv_buffer, int job_index, Variables &vars, ActiveSet &set, int &eval_id)

  lower level function shared by unpack_parameters_buffer() and unpack_parameters_initialize()

- void resolve_map1 (const String &map1, size_t &ac_index1, size_t &adi_index1, size_t &ads_index1, size_t &adr_index1, size_t curr_index, short &inactive_sm_view)

  compute variable mapping indices corresponding to map1 and update inactive view if necessary

- void resolve_real_variable_mapping (const String &map1, const String &map2, size_t curr_index, short &inactive_sm_view)

  for a named real mapping, resolve primary index and secondary target

- void resolve_integer_variable_mapping (const String &map1, const String &map2, size_t curr_index, short &inactive_sm_view)

  for a named integer mapping, resolve primary index and secondary target

- void resolve_string_variable_mapping (const String &map1, const String &map2, size_t curr_index, short &inactive_sm_view)

  for a named string mapping, resolve primary index and secondary target

- void real_variable_mapping (Real r_var, size_t av_index, short svm_target)

  insert r_var into appropriate recipient

- void integer_variable_mapping (int i_var, size_t av_index, short svm_target)

    insert i_var into appropriate recipient
- void string_variable_mapping (const String &s_var, size_t av_index, short svm_target)

    insert s_var into appropriate recipient
- void set_mapping (const ActiveSet &mapped_set, ActiveSet &interface_set, bool &opt_interface_map, ActiveSet &sub_iterator_set, bool &sub_iterator_map)

    define the evaluation requirements for the optionalInterface (interface_set) and the subIterator (sub_iterator_set) from the total model evaluation requirements (mapped_set)
- void response_mapping (const Response &interface_response, const Response &sub_iterator_response, Response &mapped_response)

    combine the response from the optional interface evaluation with the response from the sub-iteration using the primaryCoeffs/secondaryCoeffs mappings to create the total response for the model
- void interface_response_overlay (const Response &opt_interface_response, Response &mapped_response)

    assign the response from the optional interface evaluation within the total response for the model
- void iterator_response_overlay (const Response &sub_iterator_response, Response &mapped_response)

    overlay the sub-iteration response within the total response for the model using the primaryCoeffs/secondaryCoeffs mappings
- void iterator_error_estimation (const RealSymMatrix &sub_iterator_errors, RealVector &mapped_errors)

    combine error estimates from the sub-iteration to define mappedErrorEstimates
- Response & nested_response (int nested_cntr)

    locate existing or allocate new entry in nestedResponseMap
- void check_response_map (const ShortArray &mapped_asv)

    check function counts for the mapped_asv
- void update_inactive_view (short new_view, short &view)

    update inactive variables view for subIterator based on new_view
- void update_inactive_view (unsigned short type, short &view)

    update inactive variables view for subIterator based on type
- void update_sub_model (const Variables &vars, const Constraints &cons)

    update subModel with current variable values/bounds/labels

Private Attributes

- int nestedModelEvalCntr

    number of calls to derived_evaluate()/derived_evaluate_nowait()
- bool firstUpdate

    boolean to trigger one-time updates on first call to update_sub_model()
- IntResponseMap nestedResponseMap

    used to return a map of nested responses (including subIterator and optionalInterface contributions) for aggregation and rekeying at the base class level
- RealVector mappedErrorEstimates

    mapping of subIterator.response_error_estimates() through primary and secondary mappings
- size_t outerMIPLIndex

    the miPLIndex for the outer parallelism context, prior to any subIterator partitioning
- Iterator subIterator

    the sub-iterator that is executed on every evaluation of this model
- Model subModel

    the sub-model used in sub-iterator evaluations
- PRPQueue subIteratorPRPQueue

    job queue for asynchronous execution of subIterator jobs
- IteratorScheduler subIteratorSched

    scheduling object for concurrent iterator parallelism

- String subMethodPointer

    the sub-method pointer from the nested model specification
- int subIteratorJobCntr

    subIterator job counter since last synchronize()
- IntIntMap subIteratorIdMap

    mapping from subIterator evaluation counter to nested model counter (different when subIterator evaluations do not occur on every nested model evaluation due to variable ASV content)
- size_t numSubIterFns = 0

    number of sub-iterator response functions prior to mapping
- size_t numSubIterMappedIneqCon = 0

    number of top-level inequality constraints mapped from the sub-iteration results
- size_t numSubIterMappedEqCon = 0

    number of top-level equality constraints mapped from the sub-iteration results
- Interface optionalInterface

    the optional interface contributes nonnested response data to the total model response
- String optInterfacePointer

    the optional interface pointer from the nested model specification
- Response optInterfaceResponse

    the response object resulting from optional interface evaluations
- IntIntMap optInterfaceIdMap

    mapping from optionalInterface evaluation counter to nested model counter (different when optionalInterface evaluations do not occur on every nested model evaluation due to variable ASV content)
- size_t numOptInterfPrimary = 0

    number of primary response functions (objective/least squares/generic functions) resulting from optional interface evaluations
- size_t numOptInterfIneqCon = 0

    number of inequality constraints resulting from optional interface evaluations
- size_t numOptInterfEqCon = 0

    number of equality constraints resulting from the optional interface evaluations
- IntSet optInterfGradIdAnalytic

    analytic IDs for mixed gradients on the optional interface
- IntSet optInterfHessIdAnalytic

    analytic IDs for mixed Hessians on the optional interface
- String optInterfGradientType

    Gradient type for the optional interface.
- String optInterfHessianType

    Hessian type for the optional interface.
- SizetArray active1ACVarMapIndices

    "primary" variable mappings for inserting active continuous currentVariables within all continuous subModel variables. If there are no secondary mappings defined, then the insertions replace the subModel variable values.
- SizetArray active1ADIVarMapIndices

    "primary" variable mappings for inserting active discrete int currentVariables within all discrete int subModel variables. No secondary mappings are defined for discrete int variables, so the active variables replace the subModel variable values.
- SizetArray active1ADSVarMapIndices

    "primary" variable mappings for inserting active discrete string currentVariables within all discrete string subModel variables. No secondary mappings are defined for discrete string variables, so the active variables replace the subModel variable values.
- SizetArray active1ADRVarMapIndices

    "primary" variable mappings for inserting active discrete real currentVariables within all discrete real subModel variables. No secondary mappings are defined for discrete real variables, so the active variables replace the subModel variable values.
- ShortArray active2ACVarMapTargets

"secondary" variable mappings for inserting active continuous currentVariables into sub-parameters (e.g., distribution parameters for uncertain variables or bounds for continuous design/state variables) within all continuous subModel variables.

- ShortArray active2ADIVarMapTargets

  "secondary" variable mappings for inserting active discrete int currentVariables into sub-parameters (e.g., bounds for discrete design/state variables) within all discrete int subModel variables.

- ShortArray active2ADSVarMapTargets

  "secondary" variable mappings for inserting active discrete string currentVariables into sub-parameters (e.g., bounds for discrete design/state variables) within all discrete string subModel variables.

- ShortArray active2ADRVarMapTargets

  "secondary" variable mappings for inserting active discrete real currentVariables into sub-parameters (e.g., bounds for discrete design/state variables) within all discrete real subModel variables.

- SizetArray complement1ACVarMapIndices

  "primary" variable mappings for inserting the complement of the active continuous currentVariables within all continuous subModel variables

- SizetArray complement1ADIVarMapIndices

  "primary" variable mappings for inserting the complement of the active discrete int currentVariables within all discrete int subModel variables

- SizetArray complement1ADSVarMapIndices

  "primary" variable mappings for inserting the complement of the active discrete string currentVariables within all discrete string subModel variables

- SizetArray complement1ADRVarMapIndices

  "primary" variable mappings for inserting the complement of the active discrete real currentVariables within all discrete real subModel variables

- BitArray extraCVarsData

  flags for updating subModel continuous bounds and labels, one for each active continuous variable in currentVariables

- BitArray extraDIVarsData

  flags for updating subModel discrete int bounds and labels, one for each active discrete int variable in currentVariables

- BitArray extraDSVarsData

  flags for updating subModel discrete string labels, one for each active discrete string variable in currentVariables

- BitArray extraDRVarsData

  flags for updating subModel discrete real bounds and labels, one for each active discrete real variable in currentVariables

- bool identityRespMap = false

  whether identity response mapping is active

- size_t subIterMappedPri = 0

  number of sub-iterator results functions mapped to nested model primary functions (cached for use with identity case)

- size_t subIterMappedSec = 0

  number of sub-iterator results functions mapped to nested model secondary functions (cached for use with identity case)

- RealMatrix primaryRespCoeffs

  "primary" response_mapping matrix applied to the sub-iterator response functions. For OUU, the matrix is applied to UQ statistics to create contributions to the top-level objective functions/least squares/ generic response terms.

- RealMatrix secondaryRespCoeffs

  "secondary" response_mapping matrix applied to the sub-iterator response functions. For OUU, the matrix is applied to UQ statistics to create contributions to the top-level inequality and equality constraints.

Friends

- class IteratorScheduler

  protect scheduler callback functions from general access

Additional Inherited Members

14.121.1 Detailed Description

Derived model class which performs a complete sub-iterator execution within every evaluation of the model.

The NestedModel class nests a sub-iterator execution within every model evaluation. This capability is most commonly used for optimization under uncertainty, in which a nondeterministic iterator is executed on every optimization function evaluation. The NestedModel also contains an optional interface, for portions of the model evaluation which are independent from the sub-iterator, and a set of mappings for combining sub-iterator and optional interface data into a top level response for the model.

14.121.2 Member Function Documentation

14.121.2.1 void derived_evaluate (const ActiveSet & *set*) [protected], [virtual]

portion of evaluate() specific to NestedModel

Update subModel's inactive variables with active variables from currentVariables, compute the optional interface and sub-iterator responses, and map these to the total model response.

Reimplemented from Model.

References NestedModel::active2ACVarMapTargets, Response::active_set(), Interface::analysis_components(), ParallelLibrary::bcast(), ParallelLibrary::bcast_hs(), NestedModel::component_parallel_mode(), Model::currentResponse, Model::currentVariables, Interface::eval_tag_prefix(), Iterator::eval_tag_prefix(), Model::evalTagPrefix, Interface::evaluation_id(), Model::evaluationsDB, Model::hierarchicalTagging, NestedModel::interface_id(), NestedModel::interface_response_overlay(), Model::interfEvaluationsDBState, NestedModel::iterator_response_overlay(), IteratorScheduler::iteratorCommSize, IteratorScheduler::iteratorScheduling, Interface::map(), IteratorScheduler::messagePass, IteratorScheduler::miPLIndex, Model::modelId, Model::modelPCIter, NestedModel::nestedModelEvalCntr, NestedModel::optInterfaceResponse, NestedModel::optionalInterface, Model::outputLevel, ParallelLibrary::parallel_configuration_iterator(), Model::parallelLib, IteratorScheduler::peerAssignJobs, Response::reset(), Iterator::response_results(), Iterator::response_results_active_set(), Iterator::run(), IteratorScheduler::run_iterator(), NestedModel::set_mapping(), IteratorScheduler::stop_iterator_servers(), NestedModel::subIterator, NestedModel::subIteratorSched, NestedModel::update_sub_model(), and Model::userDefinedConstraints.

14.121.2.2 void derived_evaluate_nowait (const ActiveSet & *set*) [protected], [virtual]

portion of evaluate_nowait() specific to NestedModel

Asynchronous execution of subIterator on subModel and, optionally, optionalInterface.

Reimplemented from Model.

References Response::active_set(), Interface::analysis_components(), Model::currentResponse, Model::currentVariables, Interface::evaluation_id(), Model::evaluationsDB, NestedModel::interface_id(), Model::interfEvaluationsDBState, Interface::map(), Iterator::method_id(), Model::modelId, NestedModel::nestedModelEvalCntr, NestedModel::optInterfaceIdMap, NestedModel::optInterfaceResponse, NestedModel::optionalInterface, Iterator::response_results(), Iterator::response_results_active_set(), NestedModel::set_mapping(), NestedModel::subIterator, NestedModel::subIteratorIdMap, NestedModel::subIteratorJobCntr, and NestedModel::subIteratorPRPQueue.

14.121.2.3 const IntResponseMap & derived_synchronize ( ) [protected], [virtual]

portion of synchronize() specific to NestedModel

Recovery of asynchronous subIterator executions and, optionally, asynchronous optionalInterface mappings.

Reimplemented from Model.

References Interface::cache_unmatched_response(), NestedModel::component_parallel_mode(), NestedModel::interface_response_overlay(), NestedModel::iterator_response_overlay(), Model::modelPCIter, NestedModel::nested_response(), NestedModel::nestedResponseMap, IteratorScheduler::numIteratorJobs, NestedModel::optInterfaceIdMap, NestedModel::optInterfacePointer, NestedModel::optionalInterface, ParallelLibrary::parallel_configuration_iterator(), Model::parallelLib, IteratorScheduler::schedule_iterators(), NestedModel::subIterator, NestedModel::subIteratorIdMap, NestedModel::subIteratorJobCntr, NestedModel::subIteratorPRPQueue, NestedModel::subIteratorSched, and Interface::synchronize().

14.121.2.4 short local_eval_synchronization ( ) [inline], [protected], [virtual]

return optionalInterface synchronization setting

Used in setting Model::asynchEvalFlag. subModel synchronization is used for setting asynchEvalFlag within subModel.

Reimplemented from Model.

References Interface::asynch_local_evaluation_concurrency(), Interface::interface_synchronization(), NestedModel::optInterfacePointer, and NestedModel::optionalInterface.

14.121.2.5 int local_eval_concurrency ( ) [inline], [protected], [virtual]

return optionalInterface asynchronous evaluation concurrency

Used in setting Model::evaluationCapacity. subModel concurrency is used for setting evaluationCapacity within subModel.

Reimplemented from Model.

References Interface::asynch_local_evaluation_concurrency(), NestedModel::optInterfacePointer, and NestedModel::optionalInterface.

14.121.2.6 bool derived_master_overload ( ) const [inline], [protected], [virtual]

flag which prevents overloading the master with a multiprocessor evaluation (forwarded to optionalInterface)

Derived master overload for subModel is handled separately in subModel.evaluate() within subIterator.run().

Reimplemented from Model.

References Iterator::is_null(), Interface::iterator_eval_dedicated_master(), IteratorScheduler::iteratorScheduling, Interface::multi_proc_eval(), NestedModel::optInterfacePointer, NestedModel::optionalInterface, IteratorScheduler::procsPerIterator, NestedModel::subIterator, and NestedModel::subIteratorSched.

14.121.2.7 void derived_init_communicators (ParLevLIter *pl_iter*, int *max_eval_concurrency*, bool *recurse_flag* = true) [protected], [virtual]

set up optionalInterface and subModel for parallel operations

Asynchronous flags need to be initialized for the subModel. In addition, max_eval_concurrency is the outer level iterator concurrency, not the subIterator concurrency that subModel will see, and recomputing the message_lengths on the subModel is probably not a bad idea either. Therefore, recompute everything on subModel using init_communicators().

Reimplemented from Model.

References Response::active_set(), IteratorScheduler::configure(), Model::currentVariables, ProblemDescDB::get_db_method_node(), ProblemDescDB::get_db_model_node(), Interface::init_communicators(), IteratorScheduler::init_iterator(), NestedModel::init_sub_iterator(), Iterator::is_null(), IteratorScheduler::iterator_message_lengths(), IteratorScheduler::iteratorServerId, Model::messageLengths, IteratorScheduler::messagePass, Model::modelPCIter, IteratorScheduler::numIteratorServers, NestedModel::optInterfacePointer, NestedModel::optionalInterface, ParallelLibrary::parallel_configuration_iterator(), Model::parallelLib, IteratorScheduler::partition(), Model::probDescDB, MPIPackBuffer::reset(), Iterator::response_results(), ProblemDescDB::set_db_list_nodes(), ProblemDescDB::set_db_method_node(), ProblemDescDB::set_db_model_nodes(), MPIPackBuffer::size(), NestedModel::subIterator, NestedModel::subIteratorSched, NestedModel::subMethodPointer, NestedModel::subModel, and IteratorScheduler::update().

14.121.2.8 int derived_evaluation_id ( ) const [inline], [protected], [virtual]

Return the current evaluation id for the NestedModel.

return the top level nested evaluation count. To get the lower level eval count, the subModel must be explicitly queried. This is consistent with the eval counter definitions in surrogate models.

Reimplemented from Model.

References NestedModel::nestedModelEvalCntr.

14.121.2.9 void response_mapping (const Response & *opt_interface_response*, const Response & *sub_iterator_response*, Response & *mapped_response*) [inline], [private]

combine the response from the optional interface evaluation with the response from the sub-iteration using the primaryCoeffs/secondaryCoeffs mappings to create the total response for the model

```
In the OUU case,


optionalInterface fns = {f}, {g} (deterministic primary functions, constraints)
subIterator fns       = {S}      (UQ response statistics)

Problem formulation for mapped functions:
                  minimize    {f} + [W]{S}
                  subject to  {g_l} <= {g}    <= {g_u}
                              {a_l} <= [A]{S} <= {a_u}
                              {g}    == {g_t}
                              [A]{S} == {a_t}
```

where [W] is the primary_mapping_matrix user input (primaryRespCoeffs class attribute), [A] is the secondary_-mapping_matrix user input (secondaryRespCoeffs class attribute), {{g_l},{a_l}} are the top level inequality constraint lower bounds, {{g_u},{a_u}} are the top level inequality constraint upper bounds, and {{g_t},{a_t}} are the top level equality constraint targets.

NOTE: optionalInterface/subIterator primary fns (obj/lsq/generic fns) overlap but optionalInterface/subIterator secondary fns (ineq/eq constraints) do not. The [W] matrix can be specified so as to allow

- some purely deterministic primary functions and some combined: [W] filled and [W].num_rows() $<$ {f}.length() [combined first] *or* [W].num_rows() == {f}.length() and [W] contains rows of zeros [combined last]
- some combined and some purely stochastic primary functions: [W] filled and [W].num_rows() $>$ {f}.length()
- separate deterministic and stochastic primary functions: [W].num_rows() $>$ {f}.length() and [W] contains {f}.length() rows of zeros.

If the need arises, could change constraint definition to allow overlap as well: {g_l} $<=$ {g} + [A]{S} $<=$ {g_u} with [A] usage the same as for [W] above.

In the UOO case, things are simpler, just compute statistics of each optimization response function: [W] = [I], {f}/{g}/[A] are empty.

References Response::active_set_request_vector(), NestedModel::check_response_map(), NestedModel::interface_response_overlay(), and NestedModel::iterator_response_overlay().

14.121.3 Member Data Documentation

14.121.3.1 Model subModel [private]

the sub-model used in sub-iterator evaluations

There are no restrictions on subModel, so arbitrary nestings are possible. This is commonly used to support surrogate-based optimization under uncertainty by having NestedModels contain SurrogateModels and vice versa.

Referenced by NestedModel::component_parallel_mode(), NestedModel::derived_init_communicators(), NestedModel::derived_init_serial(), NestedModel::derived_subordinate_models(), NestedModel::estimate_partition_bounds(), NestedModel::fine_grained_evaluation_counters(), NestedModel::integer_variable_mapping(), NestedModel::NestedModel(), NestedModel::print_evaluation_summary(), NestedModel::real_variable_mapping(), NestedModel::resolve_integer_variable_mapping(), NestedModel::resolve_map1(), NestedModel::resolve_real_variable_mapping(), NestedModel::resolve_string_variable_mapping(), NestedModel::serve_run(), NestedModel::set_mapping(), NestedModel::string_variable_mapping(), NestedModel::subordinate_model(), NestedModel::surrogate_response_mode(), NestedModel::update_inactive_view(), NestedModel::update_sub_model(), and NestedModel::warm_start_flag().

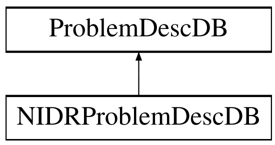
The documentation for this class was generated from the following files:

- NestedModel.hpp
- NestedModel.cpp

14.122 NIDRProblemDescDB Class Reference

The derived input file database utilizing the new IDR parser.

Inheritance diagram for NIDRProblemDescDB:



Public Member Functions

- NIDRProblemDescDB (ParallelLibrary &parallel_lib)

  constructor
- ∼NIDRProblemDescDB ()

  destructor
- void derived_parse_inputs (const std::string &dakota_input_file, const std::string &dakota_input_string, const std::string &parser_options)

  parses the input file and populates the problem description database using NIDR.
- void derived_broadcast ()

  perform any data processing that must be coordinated with DB buffer broadcasting (performed prior to broadcasting the DB buffer on rank 0 and after receiving the DB buffer on other processor ranks)
- void derived_post_process ()

  perform any additional data post-processing
- **KWH** (iface_Real)
- **KWH** (iface_Rlit)
- **KWH** (iface_false)
- **KWH** (iface_ilit)
- **KWH** (iface_int)

- **KWH** (iface_lit)
- **KWH** (iface_start)
- **KWH** (iface_stop)
- **KWH** (iface_str)
- **KWH** (iface_str2D)
- **KWH** (iface_strL)
- **KWH** (iface_true)
- **KWH** (iface_type)
- **KWH** (method_li)
- **KWH** (method_Real)
- **KWH** (method_Real01)
- **KWH** (method_RealDL)
- **KWH** (method_RealLlit)
- **KWH** (method_Realp)
- **KWH** (method_Realz)
- **KWH** (method_Ri)
- **KWH** (method_false)
- **KWH** (method_szarray)
- **KWH** (method_ilit2)
- **KWH** (method_ilit2p)
- **KWH** (method_int)
- **KWH** (method_ivec)
- **KWH** (method_lit)
- **KWH** (method_litc)
- **KWH** (method_liti)
- **KWH** (method_litp)
- **KWH** (method_litr)
- **KWH** (method_litz)
- **KWH** (method_order)
- **KWH** (method_num_resplevs)
- **KWH** (method_piecewise)
- **KWH** (method_resplevs)
- **KWH** (method_resplevs01)
- **KWH** (method_shint)
- **KWH** (method_sizet)
- **KWH** (method_slit2)
- **KWH** (method_start)
- **KWH** (method_stop)
- **KWH** (method_str)
- **KWH** (method_strL)
- **KWH** (method_true)
- **KWH** (method_tr_final)
- **KWH** (method_type)
- **KWH** (method_usharray)
- **KWH** (method_ushint)
- **KWH** (method_utype)
- **KWH** (method_augment_utype)
- **KWH** (method_utype_lit)
- **KWH** (model_Real)
- **KWH** (model_RealDL)
- **KWH** (model_ivec)
- **KWH** (model_false)
- **KWH** (model_int)
- **KWH** (model_lit)
- **KWH** (model_order)

- **KWH** (model_shint)
- **KWH** (model_sizet)
- **KWH** (model_id_to_index_set)
- **KWH** (model_start)
- **KWH** (model_stop)
- **KWH** (model_str)
- **KWH** (model_strL)
- **KWH** (model_true)
- **KWH** (model_type)
- **KWH** (model_usharray)
- **KWH** (model_ushint)
- **KWH** (model_utype)
- **KWH** (model_augment_utype)
- **KWH** (resp_RealDL)
- **KWH** (resp_RealL)
- **KWH** (resp_false)
- **KWH** (resp_intset)
- **KWH** (resp_ivec)
- **KWH** (resp_lit)
- **KWH** (resp_sizet)
- **KWH** (resp_start)
- **KWH** (resp_stop)
- **KWH** (resp_str)
- **KWH** (resp_strL)
- **KWH** (resp_true)
- **KWH** (resp_utype)
- **KWH** (resp_augment_utype)
- **KWH** (env_int)
- **KWH** (env_start)
- **KWH** (env_str)
- **KWH** (env_strL)
- **KWH** (env_true)
- **KWH** (env_utype)
- **KWH** (env_augment_utype)
- **KWH** (var_RealLb)
- **KWH** (var_RealUb)
- **KWH** (var_IntLb)
- **KWH** (var_categorical)
- **KWH** (var_caulbl)
- **KWH** (var_dauilbl)
- **KWH** (var_dauslbl)
- **KWH** (var_daurlbl)
- **KWH** (var_ceulbl)
- **KWH** (var_deuilbl)
- **KWH** (var_deuslbl)
- **KWH** (var_deurlbl)
- **KWH** (var_sizet)
- **KWH** (var_start)
- **KWH** (var_stop)
- **KWH** (var_str)
- **KWH** (var_strL)
- **KWH** (var_true)
- **KWH** (var_newiarray)
- **KWH** (var_newsarray)
- **KWH** (var_newivec)

- **KWH** (var_newrvec)
- **KWH** (var_ivec)
- **KWH** (var_svec)
- **KWH** (var_rvec)
- **KWH** (var_type)

Static Public Member Functions

- static void botch (const char ∗fmt,...)

  print and error message and immediately abort
- static void check_variables (std::list< DataVariables > ∗)

  check each node in a list of DataVariables, first mapping DataVariables members back to flat NIDR arrays if needed.
- static void **check_responses** (std::list< DataResponses > ∗)
- static void check_descriptor_format (const StringArray &labels)

  Validate format user-supplied descriptors.
- static void check_descriptors_for_repeats (const StringArray &labels)

  Ensure no response descriptors are repeated.
- static void check_descriptors_for_repeats (const StringArray &cd_labels, const StringArray &ddr_labels, const StringArray &ddsi_labels, const StringArray &ddss_labels, const StringArray &ddsr_labels, const StringArray &cs_labels, const StringArray &dsr_labels, const StringArray &dssi_labels, const StringArray &dsss_labels, const StringArray &dssr_labels, const StringArray &cau_labels, const StringArray &diau_labels, const StringArray &dsau_labels, const StringArray &drau_labels, const StringArray &ceu_labels, const StringArray &dieu_labels, const StringArray &dseu_labels, const StringArray &dreu_labels)

  Ensure no variable descriptors are repeated.
- static void make_variable_defaults (std::list< DataVariables > ∗)

  Bounds and initial point check and inferred bounds generation.
- static void **make_response_defaults** (std::list< DataResponses > ∗)
- static void squawk (const char ∗fmt,...)

  print an error message and increment nerr, but continue
- static void warn (const char ∗fmt,...)

  print a warning

Static Public Attributes

- static NIDRProblemDescDB ∗ pDDBInstance

  Pointer to the active object instance used within the static kwhandler functions in order to avoid the need for static data. Only initialized when parsing an input file; will be NULL for cases of direct DB population only.
- static int nerr = 0

  number of parse error encountered

Static Private Member Functions

- static void check_variables_node (void ∗v)

  check a single variables node; input argument v is Var_Info∗
- static int check_driver (const String &an_driver, const StringArray &link_files, const StringArray &copy_files)

  tokenize and try to validate the presence of an analysis driver, potentially included in the linked or copied template files

Private Attributes

- std::list< void ∗ > VIL

  List of Var_Info pointers, one per Variables instance.

Additional Inherited Members

14.122.1 Detailed Description

The derived input file database utilizing the new IDR parser.

The NIDRProblemDescDB class is derived from ProblemDescDB for use by the NIDR parser in processing DAKOTA input file data. For information on modifying the NIDR input parsing procedures, refer to Dakota/docs/Dev_Spec_Change.dox. For more on the parsing technology, see "Specifying and Reading Program Input with NIDR" by David M. Gay (report SAND2008-2261P, which is available in PDF form as http://dakota.sandia.gov/papers/nidr08.pdf). Source for the routines declared herein is NIDRProblemDescDB.cpp, in which most routines are so short that a description seems unnecessary.

14.122.2 Member Function Documentation

14.122.2.1 void derived_parse_inputs (const std::string & *dakota_input_file,* const std::string & *dakota_input_string,* const std::string & *parser_options*) [virtual]

parses the input file and populates the problem description database using NIDR.

Parse the input file using the Input Deck Reader (IDR) parsing system. IDR populates the IDRProblemDescDB object with the input file data.

Reimplemented from ProblemDescDB.

References Dakota::abort_handler(), NIDRProblemDescDB::botch(), ProblemDescDB::dataMethodList, DataMethodRep::dlDetails, DataMethodRep::dlLib, NIDRProblemDescDB::nerr, ProblemDescDB::parallel_library(), NIDRProblemDescDB::pDDBInstance, and NIDRProblemDescDB::squawk().

14.122.2.2 int check_driver (const String & *an_driver,* const StringArray & *link_files,* const StringArray & *copy_files*) [static], [private]

tokenize and try to validate the presence of an analysis driver, potentially included in the linked or copied template files

returns 1 if not found, 2 if found, but not executable, 0 if found (no error) in case we want to return to error on not found...

References WorkdirHelper::find_driver(), NIDRProblemDescDB::squawk(), WorkdirHelper::tokenize_driver(), NIDRProblemDescDB::warn(), and WorkdirHelper::which().

14.122.2.3 void make_variable_defaults (std::list< DataVariables > * *dvl*) [static]

Bounds and initial point check and inferred bounds generation.

Size arrays for contiguous storage of aggregated uncertain types. For each variable type, call Vgen_* to generate inferred bounds and initial point, repairing initial if needed. size the aggregate arrays for uncertain (design and state are stored separately

References Dakota::DesignAndStateLabelsCheck, NIDRProblemDescDB::squawk(), Dakota::var_mp_drange, Dakota::VLUncertainInt, Dakota::VLUncertainReal, and Dakota::VLUncertainStr.

Referenced by NIDRProblemDescDB::derived_post_process().

The documentation for this class was generated from the following files:

- NIDRProblemDescDB.hpp
- NIDRProblemDescDB.cpp

14.123 NL2Res Struct Reference

Auxiliary information passed to calcr and calcj via ur.

Public Attributes

- Real ∗ r
  residual r = r(x)
- Real ∗ J
  Jacobian J = J(x)
- Real ∗ x
  corresponding parameter vector
- int nf
  function invocation count for r(x)

14.123.1 Detailed Description

Auxiliary information passed to calcr and calcj via ur.

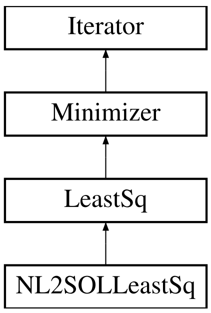
The documentation for this struct was generated from the following file:

- NL2SOLLeastSq.cpp

14.124 NL2SOLLeastSq Class Reference

Wrapper class for the NL2SOL nonlinear least squares library.

Inheritance diagram for NL2SOLLeastSq:



Public Member Functions

- NL2SOLLeastSq (ProblemDescDB &problem_db, Model &model)
  standard constructor
- NL2SOLLeastSq (Model &model)
  alternate constructor
- ∼NL2SOLLeastSq ()
  destructor
- void core_run ()
  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Static Private Member Functions

- static void calcr (int ∗np, int ∗pp, Real ∗x, int ∗nfp, Real ∗r, int ∗ui, void ∗ur, Vf vf)

  evaluator function for residual vector
- static void calcj (int ∗np, int ∗pp, Real ∗x, int ∗nfp, Real ∗J, int ∗ui, void ∗ur, Vf vf)

  evaluator function for residual Jacobian

Private Attributes

- int auxprt

  `auxilary printing bits (see Dakota Ref Manual): sum of`
  < 1 = x0prt (print initial guess) < 2 = solprt (print final solution) < 4 = statpr (print solution statistics) < 8 = parprt (print nondefault parameters) < 16 = dradpr (print bound constraint drops/adds) < debug/verbose/normal use default = 31 (everything), < quiet uses 3, silent uses 0.
- int outlev

  `frequency of output summary lines in number of iterations`
  < (debug/verbose/normal/quiet use default = 1, silent uses 0)
- Real dltfdj

  `finite-diff step size for computing Jacobian approximation`
  < (`fd_gradient_step_size`)
- Real delta0

  `finite-diff step size for gradient differences for H`
  < (a component of some covariance approximations, if desired) < (`fd_hessian_step_size`)
- Real dltfdc

  `finite-diff step size for function differences for H`
  < (`fd_hessian_step_size`)
- int mxfcal

  function-evaluation limit (`max_function_evaluations`)
- int mxiter

  iteration limit (`max_iterations`)
- Real rfctol

  relative fn convergence tolerance (`convergence_tolerance`)
- Real afctol

  absolute fn convergence tolerance (`absolute_conv_tol`)
- Real xctol

  x-convergence tolerance (`x_conv_tol`)
- Real sctol

  singular convergence tolerance (`singular_conv_tol`)
- Real lmaxs

  radius for singular-convergence test (`singular_radius`)
- Real xftol

  false-convergence tolerance (`false_conv_tol`)
- int covreq

  `kind of covariance required (\c covariance):`
  < 1 or -1 ==> sigma^2 H^-1 J^T J H^-1 < 2 or -2 ==> sigma^2 H^-1 < 3 or -3 ==> sigma^2 (J^T J)^-1 < 1 or 2 ==> use gradient diffs to estimate H < -1 or -2 ==> use function diffs to estimate H < default = 0 (no covariance)
- int rdreq

  `whether to compute the regression diagnostic vector`
  < (`regression_diagnostics`)
- Real fprec

  expected response function precision (`function_precision`)
- Real lmax0

  initial trust-region radius (`initial_trust_radius`)

Static Private Attributes

- static NL2SOLLeastSq ∗ nl2solInstance

    pointer to the active object instance used within the static evaluator functions

Additional Inherited Members

14.124.1 Detailed Description

Wrapper class for the NL2SOL nonlinear least squares library.

The NL2SOLLeastSq class provides a wrapper for NL2SOL (TOMS Algorithm 573), in the updated form of Port Library routines dn[fg][b] from Bell Labs; see http://www.netlib.org/port/readme. The Fortran from Port has been turned into C by f2c. NL2SOL uses a function pointer approach for which passed functions must be either global functions or static member functions.

14.124.2 Member Function Documentation

14.124.2.1 void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it. Details on the following subscript values appear in "Usage Summary for Selected Optimization Routines" by David M. Gay, Computing Science Technical Report No. 153, AT&T Bell Laboratories, 1990. http://netlib.bell-labs.-com/cm/cs/cstr/153.ps.gz

Reimplemented from Iterator.

References NL2SOLLeastSq::afctol, NL2SOLLeastSq::auxprt, LeastSq::bestIterPriFns, Iterator::bestVariables-Array, Minimizer::boundConstraintFlag, NL2SOLLeastSq::calcj(), NL2SOLLeastSq::calcr(), Model::continuous_-lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Dakota::copy_data(), NL2S-OLLeastSq::covreq, NL2SOLLeastSq::delta0, NL2SOLLeastSq::dltfdc, NL2SOLLeastSq::dltfdj, NL2SOLLeastSq-::fprec, Model::gradient_type(), Iterator::iteratedModel, NL2SOLLeastSq::lmax0, NL2SOLLeastSq::lmaxs, NL2S-OLLeastSq::mxfcal, NL2SOLLeastSq::mxiter, NL2SOLLeastSq::nl2solInstance, Minimizer::numContinuousVars, LeastSq::numLeastSqTerms, NL2SOLLeastSq::outlev, NL2SOLLeastSq::rdreq, LeastSq::retrievedIterPriFns, N-L2SOLLeastSq::rfctol, NL2SOLLeastSq::sctol, Minimizer::speculativeFlag, Minimizer::vendorNumericalGradFlag, NL2SOLLeastSq::xctol, and NL2SOLLeastSq::xftol.

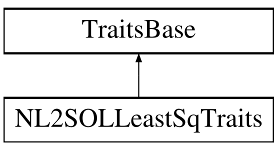
The documentation for this class was generated from the following files:

- NL2SOLLeastSq.hpp
- NL2SOLLeastSq.cpp

14.125 NL2SOLLeastSqTraits Class Reference

A version of TraitsBase specialized for NL2SOL nonlinear least squares library.

Inheritance diagram for NL2SOLLeastSqTraits:



Public Member Functions

- NL2SOLLeastSqTraits ()
  default constructor
- virtual ∼NL2SOLLeastSqTraits ()
  destructor
- virtual bool is_derived ()
  A temporary query used in the refactor.
- bool supports_continuous_variables ()
  Return the flag indicating whether method supports continuous variables.

14.125.1 Detailed Description

A version of TraitsBase specialized for NL2SOL nonlinear least squares library.

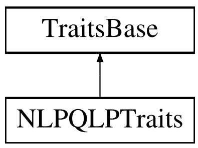
The documentation for this class was generated from the following file:

- NL2SOLLeastSq.hpp

14.126 NLPQLPTraits Class Reference

Wrapper class for the NLPQLP optimization library, Version 2.0.

Inheritance diagram for NLPQLPTraits:



Public Member Functions

- NLPQLPTraits ()
  default constructor
- virtual ∼NLPQLPTraits ()
  destructor
- virtual bool is_derived ()
  A temporary query used in the refactor.
- bool supports_continuous_variables ()
  Return the flag indicating whether method supports continuous variables.
- bool supports_linear_equality ()
  Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()
  Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()
  Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()
  Return the flag indicating whether method supports nonlinear inequalities.
- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()
  Return the format used for nonlinear inequality constraints.

14.126.1 Detailed Description

Wrapper class for the NLPQLP optimization library, Version 2.0.

```
  AN IMPLEMENTATION OF A SEQUENTIAL QUADRATIC PROGRAMMING
   METHOD FOR SOLVING NONLINEAR OPTIMIZATION PROBLEMS BY
    DISTRIBUTED COMPUTING AND NON-MONOTONE LINE SEARCH
```

This subroutine solves the general nonlinear programming problem

```
      minimize    F(X)
      subject to  G(J,X)   =  0  ,  J=1,...,ME
                  G(J,X)  >=  0  ,  J=ME+1,...,M
                  XL  <=  X  <=  XU
```

and is an extension of the code NLPQLD. NLPQLP is specifically tuned to run under distributed systems. A new input parameter L is introduced for the number of parallel computers, that is the number of function calls to be executed simultaneously. In case of L=1, NLPQLP is identical to NLPQLD. Otherwise the line search is modified to allow L parallel function calls in advance. Moreover the user has the opportunity to used distributed function calls for evaluating gradients.

The algorithm is a modification of the method of Wilson, Han, and Powell. In each iteration step, a linearly constrained quadratic programming problem is formulated by approximating the Lagrangian function quadratically and by linearizing the constraints. Subsequently, a one-dimensional line search is performed with respect to an augmented Lagrangian merit function to obtain a new iterate. Also the modified line search algorithm guarantees convergence under the same assumptions as before.

For the new version, a non-monotone line search is implemented which allows to increase the merit function in case of instabilities, for example caused by round-off errors, errors in gradient approximations, etc.

The subroutine contains the option to predetermine initial guesses for the multipliers or the Hessian of the Lagrangian function and is called by reverse communication. A version of TraitsBase specialized for NLPQLP optimizers

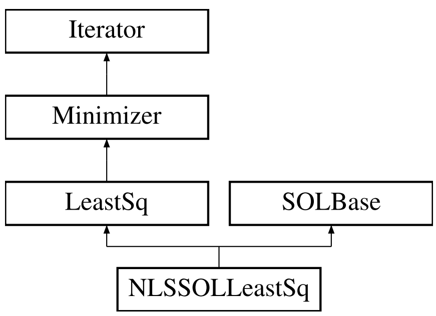
The documentation for this class was generated from the following file:

- NLPQLPOptimizer.hpp

14.127 NLSSOLLeastSq Class Reference

Wrapper class for the NLSSOL nonlinear least squares library.

Inheritance diagram for NLSSOLLeastSq:



Public Member Functions

- NLSSOLLeastSq (ProblemDescDB &problem_db, Model &model)

  standard constructor

- NLSSOLLeastSq (Model &model)

  alternate constructor
- ∼NLSSOLLeastSq ()

  destructor
- void core_run ()

  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void check_sub_iterator_conflict ()

  detect any conflicts due to recursive use of the same Fortran solver

Protected Member Functions

- void send_sol_option (std::string sol_option) override

  Resize and send option to NPSOL (npoptn) or NLSSOL (nloptn) via derived implementation.

Static Private Member Functions

- static void least_sq_eval (int &mode, int &m, int &n, int &nrowfj, double ∗x, double ∗f, double ∗gradf, int &nstate)

  Evaluator for NLSSOL: computes the values and first derivatives of the least squares terms (passed by function pointer to NLSSOL).

Static Private Attributes

- static NLSSOLLeastSq ∗ nlssolInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

14.127.1 Detailed Description

Wrapper class for the NLSSOL nonlinear least squares library.

The NLSSOLLeastSq class provides a wrapper for NLSSOL, a Fortran 77 sequential quadratic programming library from Stanford University marketed by Stanford Business Associates. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any nonstatic attribute used within static member functions must be either local to that function or accessed through a static pointer.

The user input mappings are as follows: `max_function_evaluations` is implemented directly in NLSSOLLeastSq's evaluator functions since there is no NLSSOL parameter equivalent, and `max_iterations`, `convergence_tolerance`, `output` verbosity, `verify_level`, `function_precision`, and `linesearch_tolerance` are mapped into NLSSOL's "Major Iteration Limit", "Optimality Tolerance", "Major Print Level" (`verbose:` Major Print Level = 20; `quiet:` Major Print Level = 10), "Verify Level", "Function Precision", and "Linesearch Tolerance" parameters, respectively, using NLSSOL's nloptn() subroutine (as wrapped by nloptn2() from the sol_optn_wrapper.f file). Refer to [Gill, P.E., Murray, W., Saunders, M.A., and Wright, M.H., 1986] for information on NLSSOL's optional input parameters and the nloptn() subroutine.

14.127.2 Constructor & Destructor Documentation

14.127.2.1 NLSSOLLeastSq (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This is the primary constructor. It accepts a Model reference.

References Minimizer::constraintTol, Iterator::convergenceTol, Model::fd_gradient_step_size(), ProblemDescDB::get_int(), ProblemDescDB::get_real(), Model::gradient_type(), Iterator::iteratedModel, Iterator::maxIterations, Iterator::outputLevel, Iterator::probDescDB, SOLBase::set_options(), Minimizer::speculativeFlag, and Minimizer::vendorNumericalGradFlag.

14.127.2.2 NLSSOLLeastSq (Model & *model*)

alternate constructor

This is an alternate constructor which accepts a Model but does not have a supporting method specification from the ProblemDescDB.

References Minimizer::constraintTol, Iterator::convergenceTol, Model::fd_gradient_step_size(), Model::gradient_type(), Iterator::iteratedModel, Iterator::maxIterations, Iterator::outputLevel, SOLBase::set_options(), Minimizer::speculativeFlag, and Minimizer::vendorNumericalGradFlag.

14.127.3 Member Function Documentation

14.127.3.1 void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References SOLBase::allocate_arrays(), SOLBase::allocate_workspace(), SOLBase::augment_bounds(), LeastSq::bestIterPriFns, Iterator::bestResponseArray, Iterator::bestVariablesArray, SOLBase::cLambda, SOLBase::constraint_eval(), SOLBase::constraintJacMatrixF77, SOLBase::constraintState, SOLBase::constrOffset, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Dakota::copy_data(), Dakota::copy_data_partial(), SOLBase::deallocate_arrays(), SOLBase::fnEvalCntr, SOLBase::informResult, SOLBase::intWorkSpace, SOLBase::intWorkSpaceSize, Iterator::iteratedModel, NLSSOLLeastSq::least_sq_eval(), SOLBase::linConstraintArraySize, SOLBase::linConstraintMatrixF77, Model::linear_eq_constraint_coeffs(), Model::linear_ineq_constraint_coeffs(), SOLBase::nlnConstraintArraySize, NLSSOLLeastSq::nlssolInstance, SOLBase::numberIterations, Minimizer::numContinuousVars, LeastSq::numLeastSqTerms, Minimizer::numLinearConstraints, Minimizer::numNonlinearConstraints, Minimizer::numUserPrimaryFns, SOLBase::optLSqInstance, Minimizer::prevMinInstance, SOLBase::realWorkSpace, SOLBase::realWorkSpaceSize, LeastSq::retrievedIterPriFns, SOLBase::solInstance, and SOLBase::upperFactorHessianF77.

14.127.3.2 void check_sub_iterator_conflict ( ) [virtual]

detect any conflicts due to recursive use of the same Fortran solver

This is used to avoid clashes in state between non-object-oriented (i.e., F77, C) iterator executions, when such iterators could potentially be executing simultaneously (e.g., nested execution). It is not an issue (and a used method is not reported) in cases where a helper execution is completed before a lower level one could be initiated; an example of this is DIRECT for maximization of expected improvement: the EIF maximization is completed before a new point evaluation (which could include nested iteration) is performed.

Reimplemented from Iterator.

References SOLBase::check_sub_iterator_conflict(), and Iterator::iteratedModel.

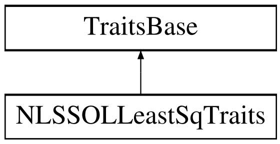
The documentation for this class was generated from the following files:

- NLSSOLLeastSq.hpp
- NLSSOLLeastSq.cpp

14.128 NLSSOLLeastSqTraits Class Reference

A version of TraitsBase specialized for NLSSOL nonlinear least squares library.

Inheritance diagram for NLSSOLLeastSqTraits:



Public Member Functions

- NLSSOLLeastSqTraits ()

    default constructor
- virtual ∼NLSSOLLeastSqTraits ()

    destructor
- virtual bool is_derived ()

    A temporary query used in the refactor.
- bool supports_continuous_variables ()

    Return the flag indicating whether method supports continuous variables.
- bool supports_linear_equality ()

    Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()

    Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()

    Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

    Return the flag indicating whether method supports nonlinear inequalities.

14.128.1 Detailed Description

A version of TraitsBase specialized for NLSSOL nonlinear least squares library.

The documentation for this class was generated from the following file:

- NLSSOLLeastSq.hpp

14.129 NoDBBaseConstructor Struct Reference

Dummy struct for overloading constructors used in on-the-fly instantiations without ProblemDescDB support.

Public Member Functions

- NoDBBaseConstructor (int=0)

    C++ structs can have constructors.

14.129.1 Detailed Description

Dummy struct for overloading constructors used in on-the-fly instantiations without ProblemDescDB support.

NoDBBaseConstructor is used to overload the constructor used for on-the-fly instantiations in which ProblemDesc-DB queries cannot be used. Putting this struct here avoids circular dependencies.

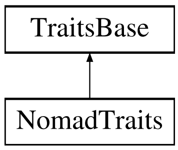
The documentation for this struct was generated from the following file:

- dakota_global_defs.hpp

14.130 NomadTraits Class Reference

Wrapper class for NOMAD Optimizer.

Inheritance diagram for NomadTraits:



Public Member Functions

- NomadTraits ()
  default constructor
- virtual ∼NomadTraits ()
  destructor
- virtual bool is_derived ()
  A temporary query used in the refactor.
- bool supports_continuous_variables ()
  Return the flag indicating whether method supports continuous variables.
- bool supports_discrete_variables ()
  Return the flag indicating whether method supports discrete variables.
- bool supports_nonlinear_equality ()
  Return the flag indicating whether method supports nonlinear equalities.
- NONLINEAR_EQUALITY_FORMAT nonlinear_equality_format ()
  Return the format used for nonlinear equality constraints.
- bool supports_nonlinear_inequality ()
  Return the flag indicating whether method supports nonlinear inequalities.
- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()
  Return the format used for nonlinear inequality constraints.

14.130.1 Detailed Description

Wrapper class for NOMAD Optimizer.

NOMAD (is a Nonlinear Optimization by Mesh Adaptive Direct search) is a simulation-based optimization package designed to efficiently explore a design space using Mesh Adaptive Search.

Mesh Adaptive Direct Search uses Meshes, discretizations of the domain space of variables. It generates multiple meshes, and as its name implies, it also adapts the refinement of the meshes in order to find the best solution of a problem.

The objective of each iteration is to find points in a mesh that improves the current solution. If a better solution is not found, the next iteration is done over a finer mesh.

Each iteration is composed of two steps: Search and Poll. The Search step finds any point in the mesh in an attempt to find an improvement; while the Poll step generates trial mesh points surrounding the current best current solution.

The NomadOptimizer is a wrapper for the NOMAD library. It features the following attributes: `max_function_evaluations`, `display_format`, `display_all_evaluations`, `function_precision`, `max_iterations`. A version of TraitsBase specialized for Nomad

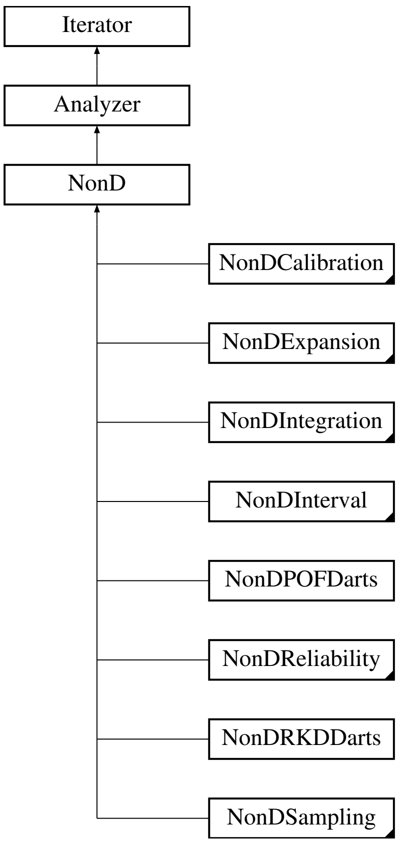
The documentation for this class was generated from the following file:

- NomadOptimizer.hpp

14.131 NonD Class Reference

Base class for all nondetermistic iterators (the DAKOTA/UQ branch).

Inheritance diagram for NonD:



Public Member Functions

- void requested_levels (const RealVectorArray &req_resp_levels, const RealVectorArray &req_prob_levels, const RealVectorArray &req_rel_levels, const RealVectorArray &req_gen_rel_levels, short resp_lev_tgt, short resp_lev_tgt_reduce, bool cdf_flag, bool pdf_output)

    set requestedRespLevels, requestedProbLevels, requestedRelLevels, requestedGenRelLevels, respLevelTarget, cdfFlag, and pdfOutput (used in combination with alternate ctors)
- void print_level_mappings (std::ostream &s) const

    prints the z/p/beta/beta∗ mappings reflected in {requested,computed}{Resp,Prob,Rel,GenRel}Levels for default qoi_type and qoi_labels

- void print_level_mappings (std::ostream &s, String qoi_type, const StringArray &qoi_labels) const

    prints the z/p/beta/beta∗ mappings reflected in {requested,computed}{Resp,Prob,Rel,GenRel}Levels
- void print_level_mappings (std::ostream &s, const RealVector &level_maps, bool moment_offset, const String &prepend="")

    print level mapping statistics using optional pre-pend
- bool resize ()

    reinitializes iterator based on new variable size
- bool pdf_output () const

    get pdfOutput
- void pdf_output (bool output)

    set pdfOutput
- short final_moments_type () const

    get finalMomentsType
- void final_moments_type (short type)

    set finalMomentsType

Protected Member Functions

- NonD (ProblemDescDB &problem_db, Model &model)

    constructor
- NonD (unsigned short method_name, Model &model)

    alternate constructor for sample generation and evaluation "on the fly"
- NonD (unsigned short method_name, const RealVector &lower_bnds, const RealVector &upper_bnds)

    alternate constructor for sample generation "on the fly"
- ∼NonD ()

    destructor
- void derived_set_communicators (ParLevLIter pl_iter)

    derived class contributions to setting the communicators associated with this Iterator instance
- void initialize_run ()

    utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers
- void finalize_run ()

    utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
- const Response & response_results () const

    return the final statistics from the nondeterministic iteration
- void response_results_active_set (const ActiveSet &set)

    set the active set within finalStatistics
- virtual void initialize_response_covariance ()

    initializes respCovariance
- virtual void initialize_final_statistics ()

    initializes finalStatistics for storing NonD final results
- virtual void update_final_statistics ()

    update finalStatistics::functionValues
- void pull_level_mappings (RealVector &level_maps, size_t offset)

    concatenate computed{Resp,Prob,Rel,GenRel}Levels into level_maps
- void push_level_mappings (const RealVector &level_maps, size_t offset)

    update computed{Resp,Prob,Rel,GenRel}Levels from level_maps
- void configure_sequence (size_t &num_steps, size_t &secondary_index, short &seq_type)

    configure fidelity/level counts from model hierarchy
- void configure_cost (unsigned short num_steps, bool multilevel, RealVector &cost)

    extract cost estimates from model hierarchy (forms or resolutions)

- bool query_cost (unsigned short num_steps, bool multilevel, RealVector &cost)

  extract cost estimates from model hierarchy, if available
- bool query_cost (unsigned short num_steps, Model &model, RealVector &cost)

  extract cost estimates from model hierarchy, if available
- bool valid_cost_values (const RealVector &cost)

  test cost for valid values > 0
- void load_pilot_sample (const SizetArray &pilot_spec, size_t num_steps, SizetArray &delta_N_l)

  distribute pilot sample specification across model forms or levels
- void load_pilot_sample (const SizetArray &pilot_spec, const Sizet3DArray &N_l, Sizet2DArray &delta_N_l)

  distribute pilot sample specification across model forms and levels
- void inflate_final_samples (const Sizet2DArray &N_l_2D, bool multilev, size_t secondary_index, Sizet3DArray &N_l_3D)

  update the relevant slice of N_l_3D from the final 2D multilevel or 2D multifidelity sample profile
- void resize_final_statistics_gradients ()

  resizes finalStatistics::functionGradients based on finalStatistics ASV
- void update_aleatory_final_statistics ()

  update finalStatistics::functionValues from momentStats and computed{Prob,Rel,GenRel,Resp}Levels
- void update_system_final_statistics ()

  update system metrics from component metrics within finalStatistics
- void update_system_final_statistics_gradients ()

  update finalStatistics::functionGradients
- void initialize_level_mappings ()

  size computed{Resp,Prob,Rel,GenRel}Levels
- void compute_densities (const RealRealPairArray &min_max_fns, bool prob_refinement=false, bool all_-levels_computed=false)

  compute the PDF bins from the CDF/CCDF values and store in computedPDF{Abscissas,Ordinates}
- void print_densities (std::ostream &s) const

  output the PDFs reflected in computedPDF{Abscissas,Ordinates} using default qoi_type and pdf_labels
- void print_densities (std::ostream &s, String qoi_type, const StringArray &pdf_labels) const

  output the PDFs reflected in computedPDF{Abscissas,Ordinates}
- void print_system_mappings (std::ostream &s) const

  print system series/parallel mappings for response levels
- void print_multilevel_evaluation_summary (std::ostream &s, const SizetArray &N_samp)

  print evaluation summary for multilevel sampling across 1D profile
- void print_multilevel_evaluation_summary (std::ostream &s, const Sizet2DArray &N_samp)

  print evaluation summary for multilevel sampling across 2D profile
- void print_multilevel_evaluation_summary (std::ostream &s, const Sizet3DArray &N_samp, String type="Final")

  print evaluation summary for multilevel sampling across 3D profile
- void construct_lhs (Iterator &u_space_sampler, Model &u_model, unsigned short sample_type, int num_-samples, int seed, const String &rng, bool vary_pattern, short sampling_vars_mode=ACTIVE)

  assign a NonDLHSSampling instance within u_space_sampler
- unsigned short sub_optimizer_select (unsigned short requested_sub_method, unsigned short default_sub_-method=SUBMETHOD_NPSOL)

  utility for vetting sub-method request against optimizers within the package configuration
- size_t one_sided_delta (Real current, Real target)

  compute a one-sided sample increment for multilevel methods to move current sampling level to a new target
- size_t one_sided_delta (const SizetArray &current, const RealVector &targets, size_t power)

  compute a one-sided sample increment for multilevel methods to move current sampling level to a new target
- size_t one_sided_delta (const SizetArray &current, Real target, size_t power)

  compute a one-sided sample increment for multilevel methods to move current sampling level to a new target

- void archive_allocate_mappings ()

  allocate results array storage for distribution mappings
- void archive_from_resp (size_t fn_index, size_t inc_id=0)

  archive the mappings from specified response levels for specified fn
- void archive_to_resp (size_t fn_index, size_t inc_id=0)

  archive the mappings to computed response levels for specified fn and (optional) increment id.
- void archive_allocate_pdf ()

  allocate results array storage for pdf histograms
- void archive_pdf (size_t fn_index, size_t inc_id=0)

  archive a single pdf histogram for specified function
- void archive_equiv_hf_evals (const Real equiv_hf_evals)

  archive the equivalent number of HF evals (used by ML/MF methods)

Protected Attributes

- NonD ∗ prevNondInstance

  pointer containing previous value of nondInstance
- size_t startCAUV

  starting index of continuous aleatory uncertain variables within active continuous variables (convenience for managing offsets)
- size_t numCAUV

  number of active continuous aleatory uncertain variables
- bool epistemicStats

  flag for computing interval-type metrics instead of integrated metrics If any epistemic vars are active in a metric evaluation, then flag is set.
- RealMatrix momentStats

  standardized or central resp moments, as determined by finalMomentsType. Calculated in compute_moments()) and indexed as (moment,fn).
- RealVectorArray requestedRespLevels

  requested response levels for all response functions
- RealVectorArray computedProbLevels

  output probability levels for all response functions resulting from requestedRespLevels
- RealVectorArray computedRelLevels

  output reliability levels for all response functions resulting from requestedRespLevels
- RealVectorArray computedGenRelLevels

  output generalized reliability levels for all response functions resulting from requestedRespLevels
- short respLevelTarget

  indicates mapping of z->p (PROBABILITIES), z->beta (RELIABILITIES), or z->beta∗ (GEN_RELIABILITIES)
- short respLevelTargetReduce

  indicates component or system series/parallel failure metrics
- RealVectorArray requestedProbLevels

  requested probability levels for all response functions
- RealVectorArray requestedRelLevels

  requested reliability levels for all response functions
- RealVectorArray requestedGenRelLevels

  requested generalized reliability levels for all response functions
- RealVectorArray computedRespLevels

  output response levels for all response functions resulting from requestedProbLevels, requestedRelLevels, or requestedGenRelLevels
- size_t totalLevelRequests

  total number of levels specified within requestedRespLevels, requestedProbLevels, and requestedRelLevels

- bool cdfFlag

  flag for type of probabilities/reliabilities used in mappings: cumulative/CDF (true) or complementary/CCDF (false)
- bool pdfOutput

  flag for managing output of response probability density functions (PDFs)
- RealVectorArray computedPDFAbscissas

  sorted response PDF intervals bounds extracted from min/max sample and requested/computedRespLevels (vector lengths = num bins + 1)
- RealVectorArray computedPDFOrdinates

  response PDF densities computed from bin counts divided by (unequal) bin widths (vector lengths = num bins)
- Response finalStatistics

  final statistics from the uncertainty propagation used in strategies: response means, standard deviations, and probabilities of failure
- short finalMomentsType

  type of moments logged within finalStatistics: none, central, standard
- size_t miPLIndex

  index for the active ParallelLevel within ParallelConfiguration::miPLIters
- BitArray pdfComputed

  Whether PDF was computed for function i; used to determine whether a pdf should be archived.

Static Protected Attributes

- static NonD ∗ nondInstance

  pointer to the active object instance used within static evaluator functions in order to avoid the need for static data

Private Member Functions

- void initialize_counts ()

  initialize data based on variable counts
- void distribute_levels (RealVectorArray &levels, bool ascending=true)

  convenience function for distributing a vector of levels among multiple response functions if a short-hand specification is employed.
- void level_mappings_file (size_t fn_index, const String &qoi_label) const

  Write level mappings to a file for a single response.
- void print_level_map (std::ostream &s, size_t fn_index, const String &qoi_label) const

  Print level mapping for a single response function to ostream.
- bool homogeneous (const SizetArray &N_l) const

  return true if N_l has consistent values

Additional Inherited Members

14.131.1 Detailed Description

Base class for all nondetermistic iterators (the DAKOTA/UQ branch).

The base class for nondeterministic iterators consolidates uncertain variable data and probabilistic utilities for inherited classes.

14.131.2 Member Function Documentation

14.131.2.1 void print_level_mappings (std::ostream & *s,* String *qoi_type,* const StringArray & *qoi_labels*) const

prints the z/p/beta/beta∗ mappings reflected in {requested,computed}{Resp,Prob,Rel,GenRel}Levels

Print distribution mappings, including to file per response.

References NonD::level_mappings_file(), Analyzer::numFunctions, Iterator::outputLevel, NonD::print_densities(), NonD::print_level_map(), NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRel-Levels, NonD::requestedRespLevels, and Dakota::write_precision.

14.131.2.2 void print_level_mappings (std::ostream & *s,* const RealVector & *level_maps,* bool *moment_offset,* const String & *prepend* = "")

print level mapping statistics using optional pre-pend

This version differs in its use of a concatenated vector of level mappings, rathen than computed{Resp,Prob,Real,Gen-Rel}Levels.

References NonD::cdfFlag, Iterator::iteratedModel, Analyzer::numFunctions, NonD::requestedGenRelLevels, Non-D::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, Model-::response_labels(), and Dakota::write_precision.

14.131.2.3 void initialize_run ( ) [inline], [protected], [virtual]

utility function to perform common operations prior to pre_run(); typically memory initialization; setting of instance pointers

Perform initialization phases of run sequence, like allocating memory and setting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's initialize_run(), typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

References Analyzer::initialize_run(), NonD::nondInstance, and NonD::prevNondInstance.

14.131.2.4 void finalize_run ( ) [inline], [protected], [virtual]

utility function to perform common operations following post_run(); deallocation and resetting of instance pointers

Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's finalize_run(), typically *after* performing its own implementation steps.

Reimplemented from Analyzer.

References Analyzer::finalize_run(), NonD::nondInstance, and NonD::prevNondInstance.

14.131.2.5 void initialize_final_statistics ( ) [protected], [virtual]

initializes finalStatistics for storing NonD final results

Default definition of virtual function (used by sampling, reliability, and stochastic expansion methods) defines the set of statistical results to include the first two moments and level mappings for each QoI.

Reimplemented in NonDInterval, and NonDEnsembleSampling.

References Dakota::abort_handler(), NonD::cdfFlag, Model::cv(), ActiveSet::derivative_vector(), NonD::epistemic-Stats, NonD::finalMomentsType, NonD::finalStatistics, Response::function_labels(), Model::inactive_continuous_-variable_ids(), Iterator::iteratedModel, Dakota::length(), Analyzer::numFunctions, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, NonD::respLevelTargetReduce, and NonD::totalLevelRequests.

Referenced by NonDEnsembleSampling::initialize_final_statistics(), NonDAdaptImpSampling::NonDAdaptImpSampling(), NonDAdaptiveSampling::NonDAdaptiveSampling(), NonDExpansion::NonDExpansion(), NonDGPImpSampling::NonDGPImpSampling(), NonDIntegration::NonDIntegration(), NonDLHSSampling::NonDLHSSampling(), NonDReliability::NonDReliability(), NonD::requested_levels(), and NonDReliability::resize().

14.131.2.6 void configure_sequence (size_t & *num_steps,* size_t & *secondary_index,* short & *seq_type*) [protected]

configure fidelity/level counts from model hierarchy

A one-dimensional sequence is assumed in this case.

References Dakota::abort_handler(), Iterator::iteratedModel, Model::multifidelity(), Model::multilevel(), Model::subordinate_models(), and Dakota::SZ_MAX.

Referenced by NonDControlVariateSampling::core_run(), NonDMultilevelSampling::core_run(), NonDExpansion::multifidelity_individual_refinement(), NonDExpansion::multifidelity_integrated_refinement(), NonDExpansion::multifidelity_reference_expansion(), NonDExpansion::multilevel_regression(), and NonDNonHierarchSampling::NonDNonHierarchSampling().

14.131.2.7 void compute_densities (const RealRealPairArray & *min_max_fns,* bool *prob_refinement =* false*,* bool *all_levels_computed =* false) [protected]

compute the PDF bins from the CDF/CCDF values and store in computedPDF{Abscissas,Ordinates}

This function infers PDFs from the CDF/CCDF level mappings, in order to enable PDF computation after CDF/CCDF probability level refinement (e.g., from importance sampling).

prob_refinement alerts the routine to exclude inverse mappings from the PDF, since refinement only applies to z->p forward mappings and mixing refined and unrefined probability mappings results in an inconsistency (potentially manifesting as negative density values).

all_levels_computed is an option used by reliability methods where computed*Levels are defined across the union of all requested levels.

References NonD::archive_allocate_pdf(), NonD::cdfFlag, NonD::computedGenRelLevels, NonD::computedPDFAbscissas, NonD::computedPDFOrdinates, NonD::computedProbLevels, NonD::computedRespLevels, Analyzer::numFunctions, NonD::pdfComputed, NonD::pdfOutput, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, and NonD::respLevelTarget.

Referenced by NonDSampling::compute_level_mappings(), NonDExpansion::compute_numerical_statistics(), NonDAdaptImpSampling::core_run(), NonDLocalReliability::core_run(), and NonDGlobalReliability::importance_sampling().

14.131.2.8 void level_mappings_file (size_t *fn_index,* const String & *qoi_label*) const [private]

Write level mappings to a file for a single response.

Write distribution mappings to a file for a single response.

References NonD::print_level_map(), and Dakota::write_precision.

Referenced by NonD::print_level_mappings().

14.131.2.9 void print_level_map (std::ostream & *s,* size_t *fn_index,* const String & *qoi_label*) const [private]

Print level mapping for a single response function to ostream.

Print the distribution mapping for a single response function to the passed output stream. This base class version maps from one requested level type to one computed level type; some derived class implementations (e.g., local and global reliability) output multiple computed level types.

References NonD::cdfFlag, NonD::computedGenRelLevels, NonD::computedProbLevels, NonD::computedRelLevels, NonD::computedRespLevels, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, and Dakota::write_precision.

Referenced by NonD::level_mappings_file(), and NonD::print_level_mappings().

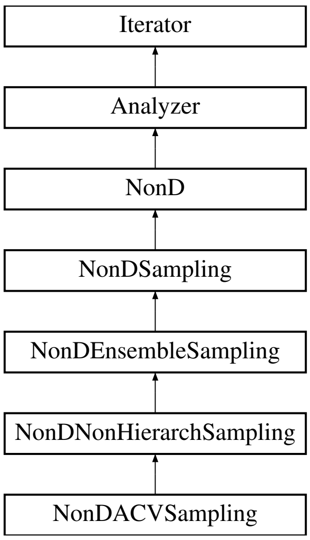
The documentation for this class was generated from the following files:

- DakotaNonD.hpp
- DakotaNonD.cpp

14.132 NonDACVSampling Class Reference

Perform Approximate Control Variate Monte Carlo sampling for UQ.

Inheritance diagram for NonDACVSampling:



Public Member Functions

- NonDACVSampling (ProblemDescDB &problem_db, Model &model)

    standard constructor
- ∼NonDACVSampling ()

    destructor

Protected Member Functions

- void core_run ()
- void approximate_control_variate ()
- void approximate_control_variate_offline_pilot ()
- void approximate_control_variate_pilot_projection ()
- void **approx_increments** (IntRealMatrixMap &sum_L_baselineH, IntRealVectorMap &sum_H, IntRealSymMatrixArrayMap &sum_LL, IntRealMatrixMap &sum_LH, const SizetArray &N_shared, const RealVector &avg_eval_ratios, Real avg_hf_target)
- bool **acv_approx_increment** (const RealVector &avg_eval_ratios, const Sizet2DArray &N_L_refined, Real hf_target, size_t iter, const SizetArray &approx_sequence, size_t start, size_t end)
- void **compute_ratios** (const RealMatrix &var_L, const RealVector &cost, RealVector &avg_eval_ratios, Real &avg_hf_target, Real &avg_estvar, Real &avg_estvar_ratio)

Private Member Functions

- void **initialize_acv_sums** (IntRealMatrixMap &sum_L_baseline, IntRealVectorMap &sum_H, IntRealSymMatrixArrayMap &sum_LL, IntRealMatrixMap &sum_LH, RealVector &sum_HH)
- void **initialize_acv_counts** (SizetArray &num_H, SizetSymMatrixArray &num_LL)
- void accumulate_acv_sums (IntRealMatrixMap &sum_L_baseline, IntRealVectorMap &sum_H, IntRealSymMatrixArrayMap &sum_LL, IntRealMatrixMap &sum_LH, RealVector &sum_HH, SizetArray &N_shared)
- void accumulate_acv_sums (RealMatrix &sum_L_baseline, RealVector &sum_H, RealSymMatrixArray &sum_LL, RealMatrix &sum_LH, RealVector &sum_HH, SizetArray &N_shared)
- void accumulate_acv_sums (IntRealMatrixMap &sum_L_baseline, IntRealSymMatrixArrayMap &sum_LL, Sizet2DArray &N_L_shared)
- void accumulate_acv_sums (IntRealMatrixMap &sum_L_refined, Sizet2DArray &N_L_refined, const SizetArray &approx_sequence, size_t approx_start, size_t approx_end)
- void **compute_LH_covariance** (const RealMatrix &sum_L_shared, const RealVector &sum_H, const RealMatrix &sum_LH, const SizetArray &N_shared, RealMatrix &cov_LH)
- void **compute_LL_covariance** (const RealMatrix &sum_L_shared, const RealSymMatrixArray &sum_LL, const SizetArray &N_shared, RealSymMatrixArray &cov_LL)
- void **covariance_to_correlation_sq** (const RealMatrix &cov_LH, const RealMatrix &var_L, const RealVector &var_H, RealMatrix &rho2_LH)
- void **compute_L_variance** (const RealMatrix &sum_L, const RealSymMatrixArray &sum_LL, const SizetArray &num_L, RealMatrix &var_L)
- void **scale_to_target** (Real avg_N_H, const RealVector &cost, RealVector &avg_eval_ratios, Real &avg_hf_target)
- Real **acv_estimator_variance** (const RealVector &avg_eval_ratios, Real avg_hf_target)
- Real **acv_estimator_variance** (const RealMatrix &eval_ratios, Real avg_N_H, const RealVector &cost, RealVector &avg_eval_ratios, Real &avg_hf_target)
- void **acv_raw_moments** (IntRealMatrixMap &sum_L_shared, IntRealMatrixMap &sum_L_refined, IntRealVectorMap &sum_H, IntRealSymMatrixArrayMap &sum_LL, IntRealMatrixMap &sum_LH, const RealVector &avg_eval_ratios, const SizetArray &N_shared, const Sizet2DArray &N_L_refined, RealMatrix &H_raw_mom)
- void **compute_acv_control** (const RealSymMatrix &cov_LL, const RealSymMatrix &F, const RealMatrix &cov_LH, size_t qoi, RealVector &beta)
- void **compute_acv_control** (RealMatrix &sum_L, Real sum_H_q, RealSymMatrix &sum_LL_q, RealMatrix &sum_LH, size_t N_shared_q, const RealSymMatrix &F, size_t qoi, RealVector &beta)
- void **update_projected_samples** (Real avg_hf_target, const RealVector &avg_eval_ratios, SizetArray &N_H_projected, Sizet2DArray &N_L_projected)

Private Attributes

- bool multiStartACV

  option for performing multiple ACV optimizations and taking the best

Additional Inherited Members

14.132.1 Detailed Description

Perform Approximate Control Variate Monte Carlo sampling for UQ.

Approximate Control Variate (ACV) is a variance-reduction technique that utilitizes lower fidelity simulations that have response QoI that are correlated with the high-fidelity response QoI.

14.132.2 Constructor & Destructor Documentation

14.132.2.1 NonDACVSampling (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), ProblemDescDB::get_ushort(), Iterator::maxFunctionEvals, NonDNonHierarchSampling::mlmfSubMethod, NonDNonHierarchSampling::optSubProblemForm, NonDNonHierarchSampling::optSubProblemSolver, Iterator::outputLevel, NonDEnsembleSampling::pilotMgmtMode, Dakota::SZ_MAX, and NonDNonHierarchSampling::truthFixedByPilot.

14.132.3 Member Function Documentation

14.132.3.1 void core_run ( ) [protected], [virtual]

The primary run function manages the general case: a hierarchy of model forms (from the ordered model fidelities within a HierarchSurrModel), each of which may contain multiple discretization levels.

Reimplemented from Iterator.

References Dakota::abort_handler(), NonDACVSampling::approximate_control_variate(), NonDACVSampling::approximate_control_variate_offline_pilot(), NonDACVSampling::approximate_control_variate_pilot_projection(), NonDNonHierarchSampling::mlmfSubMethod, NonDNonHierarchSampling::numApprox, NonDSampling::numSamples, NonDEnsembleSampling::pilotMgmtMode, and NonDEnsembleSampling::pilotSamples.

14.132.3.2 void approximate_control_variate ( ) [protected]

This function performs control variate MC across two combinations of model form and discretization level.

References NonDACVSampling::accumulate_acv_sums(), NonDEnsembleSampling::avgEstVar, NonDNonHierarchSampling::avgEstVarRatio, NonDNonHierarchSampling::covLH, NonDNonHierarchSampling::covLL, NonDEnsembleSampling::finalStatsType, NonDNonHierarchSampling::inflate(), Iterator::maxIterations, NonDEnsembleSampling::mlmfIter, Analyzer::numFunctions, NonDNonHierarchSampling::numH, NonDSampling::numSamples, NonDEnsembleSampling::numSteps, NonDEnsembleSampling::onlineCost, NonDNonHierarchSampling::recover_online_cost(), NonDEnsembleSampling::sequenceCost, and NonDEnsembleSampling::varH.

Referenced by NonDACVSampling::core_run().

14.132.3.3 void approximate_control_variate_offline_pilot ( ) [protected]

This function performs control variate MC across two combinations of model form and discretization level.

References NonDACVSampling::accumulate_acv_sums(), NonDEnsembleSampling::avgEstVar, NonDNonHierarchSampling::avgEstVarRatio, NonDNonHierarchSampling::covLH, NonDNonHierarchSampling::covLL, NonDEnsembleSampling::finalStatsType, NonDNonHierarchSampling::inflate(), NonDEnsembleSampling::mlmfIter, NonDNonHierarchSampling::numApprox, Analyzer::numFunctions, NonDNonHierarchSampling::numH, NonDSampling::numSamples, NonDEnsembleSampling::numSteps, NonDEnsembleSampling::onlineCost, NonDNonHierarchSampling::recover_online_cost(), NonDEnsembleSampling::sequenceCost, and NonDEnsembleSampling::varH.

Referenced by NonDACVSampling::core_run().

14.132.3.4 void approximate_control_variate_pilot_projection ( ) [protected]

This function performs control variate MC across two combinations of model form and discretization level.

References NonDACVSampling::accumulate_acv_sums(), NonDEnsembleSampling::avgEstVar, NonDNonHierarchSampling::avgEstVarRatio, NonDNonHierarchSampling::covLH, NonDNonHierarchSampling::covLL, NonDNonHierarchSampling::inflate(), NonDEnsembleSampling::mlmfIter, NonDNonHierarchSampling::numApprox, Analyzer::numFunctions, NonDNonHierarchSampling::numH, NonDSampling::numSamples, NonDEnsembleSampling::numSteps, NonDEnsembleSampling::onlineCost, NonDNonHierarchSampling::recover_online_cost(), NonDEnsembleSampling::sequenceCost, and NonDEnsembleSampling::varH.

Referenced by NonDACVSampling::core_run().

14.132.3.5 void accumulate_acv_sums (IntRealMatrixMap & *sum_L_baseline,* IntRealVectorMap & *sum_H,* IntRealSymMatrixArrayMap & *sum_LL,* IntRealMatrixMap & *sum_LH,* RealVector & *sum_HH,* SizetArray & *N_shared*) [private]

Multi-moment map-based version used by ACV following shared_increment()

References Analyzer::allResponses, Response::function_values(), NonDNonHierarchSampling::numApprox, and Analyzer::numFunctions.

Referenced by NonDACVSampling::approximate_control_variate(), NonDACVSampling::approximate_control_variate_offline_pilot(), and NonDACVSampling::approximate_control_variate_pilot_projection().

14.132.3.6 void accumulate_acv_sums (RealMatrix & *sum_L_baseline,* RealVector & *sum_H,* RealSymMatrixArray & *sum_LL,* RealMatrix & *sum_LH,* RealVector & *sum_HH,* SizetArray & *N_shared*) [private]

Single moment version used by offline-pilot and pilot-projection ACV following shared_increment()

References Analyzer::allResponses, Response::function_values(), NonDNonHierarchSampling::numApprox, and Analyzer::numFunctions.

14.132.3.7 void accumulate_acv_sums (IntRealMatrixMap & *sum_L_shared,* IntRealSymMatrixArrayMap & *sum_LL,* Sizet2DArray & *N_L_shared*) [private]

```
Multi-moment map-based version with fine-grained fault tolerance,
used by ACV following shared_increment()
```

void NonDACVSampling:: accumulate_acv_sums(IntRealMatrixMap& sum_L_baseline, IntRealVectorMap& sum_H, IntRealSymMatrixArrayMap& sum_LL, // L w/ itself + other L IntRealMatrixMap& sum_LH, // each L with H RealVector& sum_HH, Sizet2DArray& num_L_baseline, SizetArray& num_H, SizetSymMatrixArray& num_LL, Sizet2DArray& num_LH) { uses one set of allResponses with QoI aggregation across all Models, ordered by unorderedModels[i-1], i=1:numApprox –> truthModel

using std::isfinite; Real lf_fn, lf2_fn, hf_fn, lf_prod, lf2_prod, hf_prod; IntRespMCIter r_it; IntRVMIter h_it; IntRMMIter lb_it, lr_it, lh_it; IntRSMAMIter ll_it; int lb_ord, lr_ord, h_ord, ll_ord, lh_ord, active_ord, m; size_t qoi, approx, approx2, lf_index, lf2_index, hf_index; bool hf_is_finite;

for (r_it=allResponses.begin(); r_it!=allResponses.end(); ++r_it) { const Response& resp = r_it->second; const RealVector& fn_vals = resp.function_values(); const ShortArray& asv = resp.active_set_request_vector(); hf_index = numApprox ∗ numFunctions;

for (qoi=0; qoi<numFunctions; ++qoi, ++hf_index) { hf_fn = fn_vals[hf_index]; hf_is_finite = isfinite(hf_fn); High accumulations: if (hf_is_finite) { // neither NaN nor +/-Inf ++num_H[qoi]; High-High: sum_HH[qoi] += hf_fn ∗ hf_fn; // a single vector for ord 1 High: h_it = sum_H.begin(); h_ord = (h_it == sum_H.end()) ? 0 : h_it->first; hf_prod = hf_fn; active_ord = 1; while (h_ord) { if (h_ord == active_ord) { // support general key sequence h_it->second[qoi] += hf_prod; ++h_it; h_ord = (h_it == sum_H.end()) ? 0 : h_it->first; } hf_prod ∗= hf_fn; ++active_ord; } }

SizetSymMatrix& num_LL_q = num_LL[qoi]; for (approx=0; approx<numApprox; ++approx) { lf_index = approx ∗ numFunctions + qoi; lf_fn = fn_vals[lf_index];

Low accumulations: if (isfinite(lf_fn)) { ++num_L_baseline[approx][qoi]; ++num_LL_q(approx,approx); // Diagonal of C matrix if (hf_is_finite) ++num_LH[approx][qoi]; // pull out of moment loop lb_it = sum_L_baseline.begin(); ll_it = sum_LL.begin(); lh_it = sum_LH.begin(); lb_ord = (lb_it == sum_L_baseline.-end()) ? 0 : lb_it->first; ll_ord = (ll_it == sum_LL.end()) ? 0 : ll_it->first; lh_ord = (lh_it == sum_LH.end()) ? 0 : lh_it->first; lf_prod = lf_fn; active_ord = 1; while (lb_ord || ll_ord || lh_ord) {

Low baseline if (lb_ord == active_ord) { // support general key sequence lb_it->second(qoi,approx) += lf_prod; ++lb_it; lb_ord = (lb_it == sum_L_baseline.end()) ? 0 : lb_it->first; } Low-Low if (ll_ord == active_ord) { // support general key sequence ll_it->second[qoi](approx,approx) += lf_prod ∗ lf_prod; Off-diagonal of C matrix: look back (only) for single capture of each combination for (approx2=0; approx2<approx; ++approx2) { lf2_index = approx2 ∗ numFunctions + qoi; lf2_fn = fn_vals[lf2_index];

if (isfinite(lf2_fn)) { // both are finite if (active_ord == 1) ++num_LL_q(approx,approx2); lf2_prod = lf2_fn; for (m=1; m<active_ord; ++m) lf2_prod ∗= lf2_fn; ll_it->second[qoi](approx,approx2) += lf_prod ∗ lf2_prod; } } ++ll_it; ll_ord = (ll_it == sum_LL.end()) ? 0 : ll_it->first; } Low-High (c vector for each QoI): if (lh_ord == active_ord) { if (hf_is_finite) { hf_prod = hf_fn; for (m=1; m<active_ord; ++m) hf_prod ∗= hf_fn; lh_it->second(qoi,approx) += lf_prod ∗ hf_prod; } ++lh_it; lh_ord = (lh_it == sum_LH.end()) ? 0 : lh_it->first; }

lf_prod ∗= lf_fn; ++active_ord; } } } } } }

Single moment version with fine-grained fault tolerance, used by offline-pilot and pilot-projection ACV following shared_increment() void NonDACVSampling:: accumulate_acv_sums(RealMatrix& sum_L_baseline, RealVector& sum_H, RealSymMatrixArray& sum_LL, // L w/ itself + other L RealMatrix& sum_LH, // each L with H RealVector& sum_HH, Sizet2DArray& num_L_baseline, SizetArray& num_H, SizetSymMatrixArray& num_LL, Sizet2DArray& num_LH) { uses one set of allResponses with QoI aggregation across all Models, ordered by unorderedModels[i-1], i=1:numApprox –> truthModel

using std::isfinite; Real lf_fn, lf2_fn, hf_fn; IntRespMCIter r_it; size_t qoi, approx, approx2, lf_index, lf2_index, hf_-index; bool hf_is_finite;

for (r_it=allResponses.begin(); r_it!=allResponses.end(); ++r_it) { const Response& resp = r_it->second; const RealVector& fn_vals = resp.function_values(); const ShortArray& asv = resp.active_set_request_vector(); hf_index = numApprox ∗ numFunctions;

for (qoi=0; qoi<numFunctions; ++qoi, ++hf_index) { hf_fn = fn_vals[hf_index]; hf_is_finite = isfinite(hf_fn); High accumulations: if (hf_is_finite) { // neither NaN nor +/-Inf ++num_H[qoi]; sum_H[qoi] += hf_fn; // High sum_HH[qoi] += hf_fn ∗ hf_fn; // High-High }

SizetSymMatrix& num_LL_q = num_LL[qoi]; RealSymMatrix& sum_LL_q = sum_LL[qoi]; for (approx=0; approx<numApprox; ++approx) { lf_index = approx ∗ numFunctions + qoi; lf_fn = fn_vals[lf_index];

Low accumulations: if (isfinite(lf_fn)) { ++num_L_baseline[approx][qoi]; sum_L_baseline(qoi,approx) += lf_fn; // Low

++num_LL_q(approx,approx); // Diagonal of C matrix sum_LL_q(approx,approx) += lf_fn ∗ lf_fn; // Low-Low Off-diagonal of C matrix: look back (only) for single capture of each combination for (approx2=0; approx2<approx; ++approx2) { lf2_index = approx2 ∗ numFunctions + qoi; lf2_fn = fn_vals[lf2_index]; if (isfinite(lf2_fn)) { // both are finite ++num_LL_q(approx,approx2); sum_LL_q(approx,approx2) += lf_fn ∗ lf2_fn; } }

if (hf_is_finite) { ++num_LH[approx][qoi]; sum_LH(qoi,approx) += lf_fn ∗ hf_fn;// Low-High (c vector) } } } } } }This version used by ACV following shared_approx_increment()

References Analyzer::allResponses, Response::function_values(), NonDNonHierarchSampling::numApprox, and Analyzer::numFunctions.

14.132.3.8 void accumulate_acv_sums (IntRealMatrixMap & *sum_L_refined,* Sizet2DArray & *N_L_refined,* const SizetArray & *approx_sequence,* size_t *sequence_start,* size_t *sequence_end*) [private]

This version used by ACV following approx_increment()

References Analyzer::allResponses, Response::function_values(), and Analyzer::numFunctions.

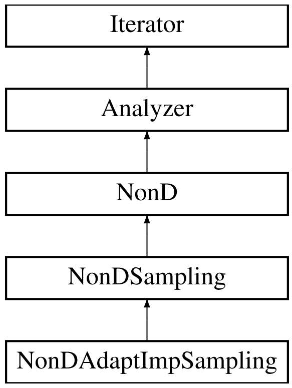
The documentation for this class was generated from the following files:

- NonDACVSampling.hpp
- NonDACVSampling.cpp

14.133 NonDAdaptImpSampling Class Reference

Class for the Adaptive Importance Sampling methods within DAKOTA.

Inheritance diagram for NonDAdaptImpSampling:



Public Member Functions

- NonDAdaptImpSampling (ProblemDescDB &problem_db, Model &model)

  standard constructor
- NonDAdaptImpSampling (Model &model, unsigned short sample_type, int samples, int seed, const String &rng, bool vary_pattern, unsigned short is_type, bool cdf_flag, bool x_space_model, bool use_model_-bounds, bool track_extreme)

  alternate constructor for on-the-fly instantiations
- ∼NonDAdaptImpSampling ()

  destructor
- bool resize ()

  reinitializes iterator based on new variable size
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

  set primaryA{CV,DIV,DRV}MapIndices, secondaryA{CV,DIV,DRV}MapTargets within derived Iterators; supports computation of higher-level sensitivities in nested contexts (e.g., derivatives of statistics w.r.t. inserted design variables)
- void core_run ()

  performs adaptive importance sampling and computes probability of failure
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final statistics
- unsigned short sampling_scheme () const

  return importanceSamplingType
- int refinement_samples () const

  return refineSamples
- void initialize (const RealVectorArray &full_points, bool x_space_data, size_t resp_index, Real initial_prob, Real failure_threshold)

initializes data needed for importance sampling: an initial set of points around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations

- void initialize (const RealMatrix &full_points, bool x_space_data, size_t resp_index, Real initial_prob, Real failure_threshold)

  initializes data needed for importance sampling: an initial set of points around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations
- void initialize (const RealVector &full_point, bool x_space_data, size_t resp_index, Real initial_prob, Real failure_threshold)

  initializes data needed for importance sampling: an initial point around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations
- Real final_probability ()

  returns the final probability calculated by the importance sampling
- const RealRealPairArray & extreme_values () const

  return extremeValues

Private Member Functions

- void select_rep_points (const RealVectorArray &var_samples_u, const RealVector &fn_samples)

  select representative points from a set of samples
- void converge_statistics (bool cov_flag)

  iteratively generate samples and select representative points until probability and (optionally) coefficient of variation converge
- void generate_samples (RealVectorArray &var_samples_u)

  generate a set of samples based on multimodal sampling density
- void evaluate_samples (const RealVectorArray &var_samples_u, RealVector &fn_samples)

  evaluate the model at the sample points and store the responses
- void calculate_statistics (const RealVectorArray &var_samples_u, const RealVector &fn_samples, size_t total_samples, Real &sum_prob, Real &prob, bool compute_cov, Real &sum_var, Real &cov)

  calculate the probability of exceeding the failure threshold and the coefficent of variation (if requested)
- Real distance (const RealVector &a, const RealVector &b)

  compute Euclidean distance between points a and b
- Real recentered_density (const RealVector &sample_point)

  compute density between a representative point and a sample point, assuming standard normal

Private Attributes

- Model uSpaceModel

  importance sampling is performed in standardized probability space. This u-space model is either passed in (alternate constructor for helper AIS) or constructed using ProbabilityTransformModel (standard constructor for stand-alone AIS)
- unsigned short importanceSamplingType

  integration type (is, ais, mmais) provided by input specification
- bool initLHS

  flag to identify if initial points are generated from an LHS sample
- bool useModelBounds

  flag to control if the sampler should respect the model bounds
- bool invertProb

  flag for inversion of probability values using 1.-p
- bool trackExtremeValues

  flag for tracking min/max values encountered when evaluating samples
- int refineSamples

  size of sample batch within each refinement iteration
- size_t respFnIndex

the active response function index in the model to be sampled

- RealVector designPoint

  design subset for which uncertain subset is being sampled
- RealVectorArray initPointsU

  the original set of u-space samples passed in initialize()
- RealVectorArray repPointsU

  the set of representative points in u-space around which to sample
- RealVector repWeights

  the weight associated with each representative point
- Real probEstimate

  the probability estimate that is iteratively refined by importance sampling
- Real failThresh

  the failure threshold (z-bar) for the problem.

Additional Inherited Members

14.133.1 Detailed Description

Class for the Adaptive Importance Sampling methods within DAKOTA.

The NonDAdaptImpSampling implements the multi-modal adaptive importance sampling used for reliability calculations. (eventually we will want to broaden this). Need to add more detail to this description.

14.133.2 Constructor & Destructor Documentation

14.133.2.1 NonDAdaptImpSampling (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This is the primary constructor. It accepts a Model reference. It will perform refinement for all response QOI and all probability levels.

References Dakota::abort_handler(), Model::assign_rep(), NonD::finalMomentsType, ProblemDescDB::get_iv(), NonD::initialize_final_statistics(), Iterator::iteratedModel, NonDSampling::numSamples, Iterator::probDescDB, NonDAdaptImpSampling::refineSamples, NonDSampling::sampleType, NonDSampling::statsFlag, NonDAdaptImpSampling::useModelBounds, and NonDAdaptImpSampling::uSpaceModel.

14.133.2.2 NonDAdaptImpSampling (Model & *model,* unsigned short *sample_type,* int *refine_samples,* int *refine_seed,* const String & *rng,* bool *vary_pattern,* unsigned short *is_type,* bool *cdf_flag,* bool *x_space_model,* bool *use_model_bounds,* bool *track_extreme*)

alternate constructor for on-the-fly instantiations

This is an alternate constructor for instantiations on the fly using a Model but no ProblemDescDB. It will perform refinement for one response QOI and one probability level (passed in initialize()).

References Model::assign_rep(), NonD::cdfFlag, NonDSampling::extremeValues, NonD::finalMomentsType, Iterator::maxEvalConcurrency, Analyzer::numFunctions, NonDAdaptImpSampling::refineSamples, NonDAdaptImpSampling::trackExtremeValues, NonDAdaptImpSampling::useModelBounds, and NonDAdaptImpSampling::uSpaceModel.

14.133.3 Member Function Documentation

14.133.3.1 void initialize (const RealVectorArray & *acv_points,* bool *x_space_data,* size_t *resp_index,* Real *initial_prob,* Real *failure_threshold*)

initializes data needed for importance sampling: an initial set of points around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations

Initializes data using a vector array of starting points.

References NonDAdaptImpSampling::designPoint, NonDAdaptImpSampling::failThresh, NonDAdaptImpSampling::initPointsU, NonDAdaptImpSampling::invertProb, NonD::numCAUV, Model::probability_transformation(), NonDAdaptImpSampling::probEstimate, NonDAdaptImpSampling::respFnIndex, NonD::startCAUV, and NonDAdaptImpSampling::uSpaceModel.

Referenced by NonDAdaptImpSampling::core_run().

14.133.3.2 void initialize (const RealMatrix & *acv_points,* bool *x_space_data,* size_t *resp_index,* Real *initial_prob,* Real *failure_threshold*)

initializes data needed for importance sampling: an initial set of points around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations

Initializes data using a matrix of starting points.

References NonDAdaptImpSampling::designPoint, NonDAdaptImpSampling::failThresh, NonDAdaptImpSampling::initPointsU, NonDAdaptImpSampling::invertProb, NonD::numCAUV, Analyzer::numContinuousVars, Model::probability_transformation(), NonDAdaptImpSampling::probEstimate, NonDAdaptImpSampling::respFnIndex, NonD::startCAUV, and NonDAdaptImpSampling::uSpaceModel.

14.133.3.3 void initialize (const RealVector & *acv_point,* bool *x_space_data,* size_t *resp_index,* Real *initial_prob,* Real *failure_threshold*)

initializes data needed for importance sampling: an initial point around which to sample, a failure threshold, an initial probability to refine, and flags to control transformations

Initializes data using only one starting point.

References NonDAdaptImpSampling::designPoint, NonDAdaptImpSampling::failThresh, NonDAdaptImpSampling::initPointsU, NonDAdaptImpSampling::invertProb, NonD::numCAUV, Model::probability_transformation(), NonDAdaptImpSampling::probEstimate, NonDAdaptImpSampling::respFnIndex, NonD::startCAUV, and NonDAdaptImpSampling::uSpaceModel.

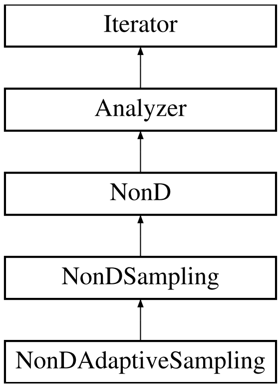
The documentation for this class was generated from the following files:

- NonDAdaptImpSampling.hpp
- NonDAdaptImpSampling.cpp

14.134 NonDAdaptiveSampling Class Reference

Class for testing various Adaptively sampling methods using geometric, statisctical, and topological information of the surrogate.

Inheritance diagram for NonDAdaptiveSampling:



Public Member Functions

- NonDAdaptiveSampling (ProblemDescDB &problem_db, Model &model)

    standard constructor
- ∼NonDAdaptiveSampling ()

    alternate constructor for sample generation and evaluation "on the fly" has not been implemented
- bool resize ()

    reinitializes iterator based on new variable size

Protected Member Functions

- void derived_init_communicators (ParLevLIter pl_iter)

    derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

    derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

    derived class contributions to freeing the communicators associated with this Iterator instance
- void core_run ()

    core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- Real **final_probability** ()
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

    print the final iterator results

Private Member Functions

- void calc_score_alm ()

    Function to compute the ALM scores for the candidate points ALM score is the variance computed by the surrogate at the point.
- void calc_score_delta_x ()

    Function to compute the Distance scores for the candidate points Distance score is the shortest distance between the candidate and an existing training point.
- void calc_score_delta_y ()

    Function to compute the Gradient scores for the candidate points Gradient score is the function value difference between a candidate's surrogate response and its nearest evaluated true response from the training set.
- void calc_score_topo_bottleneck ()

    Function to compute the Bottleneck scores for the candidate points Bottleneck score is computed by determining the bottleneck distance between the persistence diagrams of two approximate Morse-Smale complices. The complices used include one built from only the training data, and another built from the training data and the single candidate.
- void calc_score_topo_avg_persistence (int respFnCount)

Function to compute the Average Change in Persistence scores for the candidate points Avg_Persistence score is computed as the average change in persistence each point undergoes between two approximate Morse-Smale complices. The complices used include one built from only the training data, and another built from the training data and the single candidate.

- void calc_score_topo_highest_persistence (int respFnCount)

  Function to compute the Highest Persistence scores for the candidate points Highest Persistence score is calculated as a ranking of a set of candidates by constructing an approximate Morse-Smale complex over the entire set of candidates, using their surrogate responses, and the training data, using their true responses, and ranking points based on the most topological significance as measured by their persistence values. In the case where there are no topologically significant points, the point will be chosen randomly TODO: It may be wiser to fall back to a scheme that ranks points based on proximity to extrema, or the most significant extream?
- void calc_score_topo_alm_hybrid (int respFnCount)

  Function to comptue the Hybrid scores for the candidate points Hybrid score is computed the same as Avg_-Persistence score except that instead of computing one score, three scores are computing not only a mean surface, but a mean +/- std. dev. surfaces and then averaging the three separate scores. The hope is that you strike a balance between selecting points in topologically important areas and areas of high uncertainty.
- Real calc_score_alm (int respFnCount, RealVector &test_point)

  Same as the otehr function of the same name, only this allows the user to specify the location of the candidate.
- Real calc_score_delta_x (int respFnCount, RealVector &test_point)

  Same as the otehr function of the same name, only this allows the user to specify the location of the candidate.
- Real calc_score_delta_y (int respFnCount, RealVector &test_point)

  Same as the otehr function of the same name, only this allows the user to specify the location of the candidate.
- Real calc_score_topo_bottleneck (int respFnCount, RealVector &test_point)

  Same as the otehr function of the same name, only this allows the user to specify the location of the candidate.
- Real calc_score_topo_avg_persistence (int respFnCount, RealVector &test_point)

  Same as the otehr function of the same name, only this allows the user to specify the location of the candidate.
- Real calc_score_topo_alm_hybrid (int respFnCount, RealVector &test_point)

  Same as the otehr function of the same name, only this allows the user to specify the location of the candidate.
- Real compute_rmspe ()

  Using the validationSet, compute the RMSE over the surface.
- void compare_complices (int dim, std::ostream &output)

  Using the validationSet, compute the approximate Morse-Smale complices of the true model over the validationSet as well as the surrogate model over the validationSet, and output some topological comparisons.
- void parse_options ()

  Parse misc_options specified in a user input deck.
- RealVectorArray drawNewX (int this_k, int respFnCount=0)

  function to pick the next X value to be evaluated by the Iterated model
- void output_round_data (int round, int respFnCount=0)

  Temporary function for dumping validation data to output files to be visualized in TopoAS.
- void update_amsc (int respFnCount=0)

  Update the approximate Morse-Smale complex based on the training points and selected candidates. Uses surrogate function responses.
- void construct_fsu_sampler (Iterator &u_space_sampler, Model &u_model, int num_samples, int seed, unsigned short sample_type)

  Copy of construct_lhs only it allows for the construction of FSU sample designs. This can break the fsu_cvt, so it is not used at the moment, and these designs only affect the initial sample build not the candidate sets constructed at each round.
- void output_for_optimization (int dim)

  This function will write an input deck for a multi-start global optimization run of DAKOTA by extracting all of the local minima off the approximate Morse-Smale complex created from the validation set of the surrogate model.
- Real median (const RealVector &sorted_data)

  compute the median of the sorted values passed in
- void pick_new_candidates ()

  Pick new candidates from Emulator.
- void score_new_candidates ()

  Score New candidates based on the chosen metrics.

Private Attributes

- Iterator gpBuild

  LHS iterator for building the initial GP.
- Iterator gpEval

  LHS iterator for sampling on the GP.
- Iterator gpFinalEval

  LHS iterator for sampling on the final GP.
- Model gpModel

  GP model of response, one approximation per response function.
- int numRounds

  the number of rounds of additions of size batchSize to add to the original set of LHS samples
- int numPtsTotal

  the total number of points
- int numEmulEval

  the number of points evaluated by the GP each iteration
- int numFinalEmulEval

  number of points evaluated on the final GP
- int scoringMethod

  the type of scoring metric to use for sampling
- Real finalProb

  the final calculated probability (p)
- RealVectorArray gpCvars

  Vector to hold the current values of the current sample inputs on the GP.
- RealVectorArray gpMeans

  Vector to hold the current values of the current mean estimates for the sample values on the GP.
- RealVectorArray gpVar

  Vector to hold the current values of the current variance estimates for the sample values on the GP.
- RealVector emulEvalScores

  Vector to hold the scored values for the current GP samples.
- RealVector predictionErrors

  Vector to hold the RMSE after each round of adaptively fitting the model.
- RealVectorArray validationSet

  Validation point set used to determine predictionErrors above.
- RealVector yTrue

  True function responses at the values corresponding to validationSet.
- RealVector yModel

  Surrogate function responses at the values corresponding to validationSet.
- int validationSetSize

  Number of points used in the validationSet.
- int batchSize

  Number of points to add each round, default = 1.
- String batchStrategy

  String describing the tpye of batch addition to use. Allowable values are naive, distance, topology.
- String outputDir

  Temporary string for dumping validation files used in TopoAS visualization.
- String scoringMetric

  String describing the method for scoring candidate points. Options are: alm, distance, gradient, highest_persistence, avg_persistence, bottleneck, alm_topo_hybrid Note: alm and alm_topo_hybrid will fail when used with surrogates other than global_kriging as it is based on the variance of the surrogate. At the time of implementation, global_kriging is the only surrogate capable of yielding this information.
- unsigned short sampleDesign

enum describing the initial sample design. Options are: RANDOM_SAMPLING, FSU_CVT, FSU_HALTON, FSU_HAMMERSLEY

- String approx_type

  String describing type of surrogate is used to fit the data. Options are: global_kriging, global_mars, global_neural_network, global_polynomial, globabl_moving_least_squares, global_radial_basis.

- MS_Complex ∗ AMSC

  The approximate Morse-Smale complex data structure.

- int numKneighbors

  The number of approximate nearest neighbors to use in computing the AMSC.

- bool outputValidationData

  Temporary variable for toggling writing of data files to be used by TopoAS.

Additional Inherited Members

14.134.1 Detailed Description

Class for testing various Adaptively sampling methods using geometric, statisctical, and topological information of the surrogate.

NonDAdaptiveSampling implements an adaptive sampling method based on the work presented in Adaptive Sampling with Topological Scores by Dan Maljovec, Bei Wang, Ana Kupresanin, Gardar Johannesson, Valerio Pascucci, and Peer-Timo Bremer presented in IJUQ (insert issue). The method computes scores based on the topology of the known data and the topology of the surrogate model. A number of alternate adaption strategies are offered as well.

14.134.2 Constructor & Destructor Documentation

14.134.2.1 NonDAdaptiveSampling (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

```
This constructor is called for a standard letter-envelope iterator
```

instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), Response::active_set(), NonDAdaptiveSampling::AMSC, NonDAdaptiveSampling::approx_type, Iterator::assign_rep(), Model::assign_rep(), NonDAdaptiveSampling::batchSize, NonDAdaptiveSampling::batchStrategy, NonDAdaptiveSampling::construct_fsu_sampler(), NonD::construct_lhs(), Model::current_response(), ProblemDescDB::get_bool(), ProblemDescDB::get_int(), ProblemDescDB::get_iv(), ProblemDescDB::get_sa(), ProblemDescDB::get_string(), ProblemDescDB::get_ushort(), NonDAdaptiveSampling::gpBuild, NonDAdaptiveSampling::gpEval, NonDAdaptiveSampling::gpFinalEval, NonDAdaptiveSampling::gpModel, Model::gradient_type(), Model::hessian_type(), NonD::initialize_final_statistics(), Iterator::iteratedModel, Iterator::maxIterations, NonDAdaptiveSampling::numEmulEval, NonDAdaptiveSampling::numFinalEmulEval, NonDAdaptiveSampling::numKneighbors, NonDAdaptiveSampling::numRounds, NonDSampling::numSamples, NonDAdaptiveSampling::outputDir, Iterator::outputLevel, NonDAdaptiveSampling::outputValidationData, NonDAdaptiveSampling::parse_options(), Iterator::probDescDB, NonDSampling::randomSeed, ActiveSet::request_values(), NonDSampling::rngName, NonDAdaptiveSampling::sampleDesign, NonDSampling::sampleType, NonDAdaptiveSampling::scoringMetric, NonDSampling::vary_pattern(), and NonDSampling::varyPattern.

14.134.2.2 ∼NonDAdaptiveSampling ( )

alternate constructor for sample generation and evaluation "on the fly" has not been implemented

destructor

14.134.3 Member Function Documentation

14.134.3.1 void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Iterator::all_responses(), Model::append_approximation(), Model::approximation_data(), NonDAdaptiveSampling::batchSize, Model::build_approximation(), NonDAdaptiveSampling::compare_complices(), NonDAdaptiveSampling::compute_rmspe(), NonD::computedProbLevels, Model::continuous_variables(), Model::current_response(), Model::current_variables(), NonDAdaptiveSampling::drawNewX(), Model::evaluate(), Model::evaluation_id(), NonDAdaptiveSampling::gpCvars, NonDAdaptiveSampling::gpFinalEval, NonDAdaptiveSampling::gpMeans, NonDAdaptiveSampling::gpModel, NonDAdaptiveSampling::gpVar, NonD::initialize_level_mappings(), Iterator::iteratedModel, Iterator::methodPCIter, NonD::miPLIndex, NonDAdaptiveSampling::numEmulEval, NonDAdaptiveSampling::numFinalEmulEval, Analyzer::numFunctions, NonDAdaptiveSampling::numPtsTotal, NonDAdaptiveSampling::numRounds, NonDSampling::numSamples, NonDAdaptiveSampling::output_round_data(), NonDAdaptiveSampling::pick_new_candidates(), NonDAdaptiveSampling::predictionErrors, NonD::requestedRespLevels, Iterator::run(), NonDAdaptiveSampling::score_new_candidates(), NonDAdaptiveSampling::scoringMetric, and NonDAdaptiveSampling::update_amsc().

14.134.3.2 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

References NonD::print_level_mappings(), and NonDSampling::statsFlag.

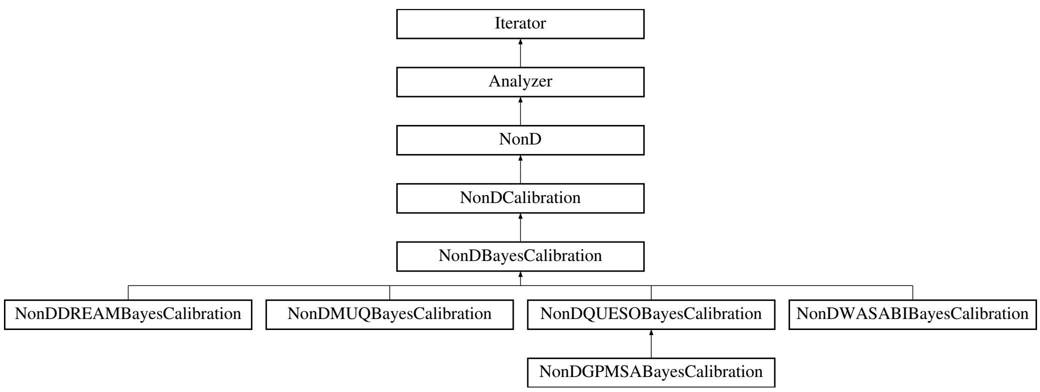
The documentation for this class was generated from the following files:

- NonDAdaptiveSampling.hpp
- NonDAdaptiveSampling.cpp

14.135 NonDBayesCalibration Class Reference

Base class for Bayesian inference: generates posterior distribution on model parameters given experimental data.

Inheritance diagram for NonDBayesCalibration:



Public Member Functions

- NonDBayesCalibration (ProblemDescDB &problem_db, Model &model)

    standard constructor
- ∼NonDBayesCalibration ()

    destructor
- template<typename VectorType >
  Real prior_density (const VectorType &vec)

    compute the prior PDF for a particular MCMC sample
- template<typename VectorType >
  Real log_prior_density (const VectorType &vec)

    compute the log prior PDF for a particular MCMC sample
- template<typename Engine >
  void prior_sample (Engine &rng, RealVector &prior_samples)

    draw a multivariate sample from the prior distribution
- template<typename VectorType >
  void prior_mean (VectorType &mean_vec) const

    return the mean of the prior distribution
- template<typename MatrixType >
  void prior_variance (MatrixType &var_mat) const

    return the covariance of the prior distribution
- template<>
  Real **prior_density** (const RealVector &vec)
- template<>
  Real **log_prior_density** (const RealVector &vec)

Static Public Member Functions

- static void get_positive_definite_covariance_from_hessian (const RealSymMatrix &hessian, const RealMatrix &prior_chol_fact, RealSymMatrix &covariance, short output_lev)

    Compute the proposal covariance C based on low-rank approximation to the prior-preconditioned misfit Hessian.
- static Real **knn_kl_div** (RealMatrix &distX_samples, RealMatrix &distY_samples, size_t dim)
- static Real **knn_mutual_info** (RealMatrix &Xmatrix, int dimX, int dimY, unsigned short alg)

Protected Member Functions

- void pre_run ()

    pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()

    core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void derived_init_communicators (ParLevLIter pl_iter)

    derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

    derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

    derived class contributions to freeing the communicators associated with this Iterator instance
- virtual void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

    print the final iterator results
- void print_variables (std::ostream &s, const RealVector &c_vars)

    convenience function to print calibration parameters, e.g., for MAP / best parameters
- const Model & algorithm_space_model () const

- virtual void specify_prior ()

  Methods for instantiating a Bayesian inverse problem. No-ops in the base class that can be specialized by child classes.
- virtual void **specify_likelihood** ()
- virtual void **init_bayesian_solver** ()
- virtual void **specify_posterior** ()
- virtual void calibrate ()=0

  Perform Bayesian calibration (all derived classes must implement)
- void construct_mcmc_model ()

  construct mcmcModel (no emulation, GP, PCE, or SC) that wraps inbound Model
- void init_hyper_parameters ()

  initialize the hyper-parameter priors
- void init_map_optimizer ()

  initialize the MAP optimizer selection
- void construct_map_model ()

  construct the negative log posterior RecastModel (negLogPostModel)
- void construct_map_optimizer ()

  construct the MAP optimizer for minimization of negLogPostModel
- virtual void map_pre_solve ()
- void initialize_model ()

  initialize emulator model and probability space transformations
- void calibrate_with_adaptive_emulator ()

  Run calibration, looping to refine emulator around posterior mode.
- virtual void filter_chain_by_conditioning ()

  Filter mcmc chain for PCE adaptive emulator. extract batchSize points from the MCMC chain and store final aggregated set within allSamples; unique points with best conditioning are selected, as determined by pivoted LU.
- void best_to_all ()

  copy bestSamples to allSamples to use in surrogate update
- void update_model ()

  evaluates allSamples on iteratedModel and update the mcmcModel emulator with all{Samples,Responses}
- Real assess_emulator_convergence ()

  compute the L2 norm of the change in emulator coefficients
- void calibrate_to_hifi ()

  calibrate the model to a high-fidelity data source, using mutual information-guided design of experiments (adaptive experimental design)
- void eval_hi2lo_stop (bool &stop_metric, double &prev_MI, const RealVector &MI_vec, int num_hifi, int max_hifi, int num_candidates)

  evaluate stopping criteria for calibrate_to_hifi
- void print_hi2lo_file (std::ostream &out_file, int num_it, const VariablesArray &optimal_config_matrix, const RealVector &MI_vec, RealMatrix &resp_matrix)

  print calibrate_to_hifi progress to file
- void print_hi2lo_begin (int num_it)

  print calibrate_to_hifi progress
- void **print_hi2lo_status** (int num_it, int i, const Variables &xi_i, double MI)
- void **print_hi2lo_batch_status** (int num_it, int batch_n, int batchEvals, const Variables &optimal_config, double max_MI)
- void **print_hi2lo_selected** (int num_it, const VariablesArray &optimal_config_matrix, const RealVector &MI_vec)
- void **print_hi2lo_chain_moments** ()
- void add_lhs_hifi_data ()

  supplement high-fidelity data with LHS samples
- void choose_batch_from_mutual_info (int random_seed, int num_it, int max_hifi, int num_hifi, RealMatrix &mi_chain, VariablesArray &design_matrix, VariablesArray &optimal_config_matrix, RealVector &MI_vec)

calculate the optimal points to add for a given batch

- void apply_hifi_sim_error (int &random_seed, int num_exp, int exp_offset=0)

  apply simulation error vector

- void **apply_error_vec** (const RealVector &error_vec, int &seed, int experiment)
- void build_error_matrix (const RealVector &sim_error_vec, RealMatrix &sim_error_matrix, int &seed)

  build matrix of errors

- void build_designs (VariablesArray &design_matrix)

  build matrix of candidate points

- void build_hi2lo_xmatrix (RealMatrix &Xmatrix, int i, const RealMatrix &mi_chain, RealMatrix &sim_error_-matrix)

  build matrix to calculate mutual information for calibrate_to_hifi

- void run_hifi (const VariablesArray &optimal_config_matrix, RealMatrix &resp_matrix)

  run high-fidelity model at several configs and add to experiment data

- void build_model_discrepancy ()

  calculate model discrepancy with respect to experimental data

- void **build_scalar_discrepancy** ()
- void **build_field_discrepancy** ()
- void **build_GP_field** (const RealMatrix &t, RealMatrix &t_pred, const RealVector &concat_disc, RealVector &disc_pred, RealVector &disc_var)
- void calculate_kde ()

  calculate a Kernel Density Estimate (KDE) for the posterior samples

- void calculate_evidence ()

  calculate the model evidence

- void **extract_selected_posterior_samples** (const std::vector< int > &points_to_keep, const RealMatrix &samples_for_posterior_eval, const RealVector &posterior_density, RealMatrix &posterior_data) const
- void **export_posterior_samples_to_file** (const std::string filename, const RealMatrix &posterior_data) const

- template<typename VectorType1 , typename VectorType2 >
  void augment_gradient_with_log_prior (VectorType1 &log_grad, const VectorType2 &vec)

  compute the (approximate) gradient of the negative log posterior by augmenting the (approximate) gradient of the negative log likelihood with the gradient of the negative log prior

- template<typename MatrixType , typename VectorType >
  void augment_hessian_with_log_prior (MatrixType &log_hess, const VectorType &vec)

  compute the (approximate) Hessian of the negative log posterior by augmenting the (approximate) Hessian of the negative log likelihood with the Hessian of the negative log prior

- Real log_likelihood (const RealVector &residuals, const RealVector &hyper_params)

  calculate log-likelihood from the passed residuals (assuming they are already sized and scaled by covariance / hyperparams...

- void prior_cholesky_factorization ()

  compute priorCovCholFactor based on prior distributions for random variables and any hyperparameters

- void get_positive_definite_covariance_from_hessian (const RealSymMatrix &hessian, RealSymMatrix &co-variance)

  member version forwards member data to static function

- void scale_model ()

  Wrap iteratedModel in a RecastModel that performs response scaling.

- void weight_model ()

  Wrap iteratedModel in a RecastModel that weights the residuals.

- void export_discrepancy (RealMatrix &pred_config_mat)

  print tabular files containing model+discrepancy responses and variances

- void export_field_discrepancy (RealMatrix &pred_vars_mat)

  print tabular files containing model+discrepancy responses and variances for field responses

- virtual void compute_statistics ()

  Compute final stats for MCMC chains.

- void export_chain ()

  export the acceptance chain in user space
- void export_chain (RealMatrix &filtered_chain, RealMatrix &filtered_fn_vals)

  Print filtered posterior and function values (later: credibility and prediction intervals)
- void filter_chain (const RealMatrix &acceptance_chain, RealMatrix &filtered_chain, int target_length)

  Perform chain filtering based on target chain length.
- void filter_chain (const RealMatrix &acceptance_chain, RealMatrix &filtered_chain)

  Perform chain filtering with burn-in and sub-sampling.
- void **filter_fnvals** (const RealMatrix &accepted_fn_vals, RealMatrix &filtered_fn_vals)
- void filter_matrix_cols (const RealMatrix &orig_matrix, int start_index, int stride, RealMatrix &filtered_matrix)

  return a newly allocated filtered matrix including start_index and every stride-th index after; for burn-in cases, start_-index is the number of burn-in discards
- void **compute_intervals** ()
- void **compute_prediction_vals** (RealMatrix &filtered_fn_vals, RealMatrix &PredVals, int num_filtered, size_t num_exp, size_t num_concatenated)
- void **print_intervals_file** (std::ostream &stream, RealMatrix &functionvalsT, RealMatrix &predvalsT, int length, size_t aug_length)
- void **print_intervals_screen** (std::ostream &stream, RealMatrix &functionvalsT, RealMatrix &predvalsT, int length)
- void kl_post_prior (RealMatrix &acceptanceChain)

  Compute information metrics.
- void **prior_sample_matrix** (RealMatrix &prior_dist_samples)
- void **mutual_info_buildX** ()
- void **print_kl** (std::ostream &stream)
- void **print_chain_diagnostics** (std::ostream &s)
- void **print_batch_means_intervals** (std::ostream &s)

Static Protected Member Functions

- static void neg_log_post_resp_mapping (const Variables &model_vars, const Variables &nlpost_vars, const Response &model_resp, Response &nlpost_resp)

  static function passed by pointer to negLogPostModel recast model
- static void **ann_dist** (const ANNpointArray matrix1, const ANNpointArray matrix2, RealVector &distances, int NX, int NY, int dim2, IntVector &k, double eps)
- static void **ann_dist** (const ANNpointArray matrix1, const ANNpointArray matrix2, RealVector &distances, Int2DArray &indices, int NX, int NY, int dim2, IntVector &k, double eps)

Protected Attributes

- String **scalarDataFilename**
- short emulatorType

  the emulator type: NO_EMULATOR, GP_EMULATOR, PCE_EMULATOR, SC_EMULATOR, ML_PCE_EMULATO-R, MF_PCE_EMULATOR, or MF_SC_EMULATOR
- RealVectorArray prevCoeffs

  cache previous expansion coefficients for assessing convergence of emulator refinement process
- Model mcmcModel

  Model instance employed in the likelihood function; provides response function values from Gaussian processes, stochastic expansions (PCE/SC), or direct access to simulations (no surrogate option)
- bool mcmcModelHasSurrogate

  whether the MCMC Model is a surrogate, or a thin transformation around a surrogate, so can be cheaply re-evaluated in chain recovery
- Model residualModel

  DataTransformModel wrapping the mcmcModel.

- Iterator mapOptimizer

  SQP or NIP optimizer for pre-solving for the MAP point prior to MCMC. This is restricted to emulator cases for now, but as for derivative preconditioning, could be activated for no-emulator cases with a specification option (not active by default).
- Model negLogPostModel

  RecastModel for solving for MAP: reduces residualModel to scalar negative log posterior.
- unsigned short mapOptAlgOverride

  user setting of the MAP optimization algorithm type
- Iterator stochExpIterator

  NonDPolynomialChaos or NonDStochCollocation instance for defining a PCE/SC-based mcmcModel.
- int chainSamples

  number of samples in the chain (e.g. number of MCMC samples); for iterative update cycles, number of samples per update cycle
- int randomSeed

  random seed for MCMC process
- unsigned int batchSize

  number of points to add to surrogate at each iteration of calibrate_with_adaptive_emulator
- short mcmcDerivOrder

  order of derivatives used in MCMC process (bitwise like ASV)
- RealVector mapSoln

  solution for most recent MAP pre-solve; also serves as initial guess for initializing the first solve and warm-starting the next solve (posterior emulator refinement)
- bool adaptExpDesign

  whether to perform iterative design of experiments with high-fidelity model
- size_t numCandidates

  number of candidate designs for adaptive Bayesian experimental design
- String importCandPtsFile

  whether to import candidate design points for adaptive Bayesian experimental design
- unsigned short importCandFormat

  tabular format for the candidate design points import file
- int maxHifiEvals

  maximum number of high-fidelity model runs to be used for adaptive Bayesian experimental design
- int batchEvals

  number of optimal designs selected per iteration of experimental design algorithm
- unsigned short mutualInfoAlg

  algorithm to employ in calculating mutual information
- bool readFieldCoords

  need field coordinates for model discrepancy
- bool calModelDiscrepancy

  flag whether to calculate model discrepancy
- String discrepancyType

  set discrepancy type
- String exportCorrModelFile

  filename for corrected model (model+discrepancy) calculations output
- String exportDiscrepFile

  filename for discrepancy calculations output
- String exportCorrVarFile

  filename for corrected model variance calculations
- unsigned short exportCorrModelFormat

  format options for corrected model output
- unsigned short exportDiscrepFormat

format options for discrepancy output

- unsigned short exportCorrVarFormat

  format options for corrected model variance output
- short discrepPolyOrder

  specify polynomial or trend order for discrepancy correction
- size_t numPredConfigs

  number of prediction configurations at which to calculate model discrepancy
- RealVector configLowerBnds

  lower bounds on configuration domain
- RealVector configUpperBnds

  upper bounds on configuration domain
- ResponseArray discrepancyResponses

  array containing predicted of model+discrepancy
- ResponseArray correctedResponses

  array containing predicted of model+discrepancy
- RealMatrix correctedVariances

  matrix containing variances of model+discrepancy
- RealVector predictionConfigList

  list of prediction configurations at which to calculate model discrepancy
- String importPredConfigs

  whether to import prediction configurations at which to calculate model discrepancy
- unsigned short importPredConfigFormat

  tabular format for prediction configurations import file
- RealVector discrepancyFieldResponses

  array containing predicted of model+discrepancy
- RealVector correctedFieldResponses

  array containing predicted of model+discrepancy
- RealVector correctedFieldVariances

  matrix containing variances of model+discrepancy
- Model hifiModel

  a high-fidelity model data source (given by pointer in input)
- int initHifiSamples

  initial high-fidelity model samples
- Iterator hifiSampler

  LHS iterator to generate hi-fi model data.
- RealMatrix priorCovCholFactor

  the Cholesky factor of the prior covariance
- unsigned short obsErrorMultiplierMode

  mode for number of observation error multipliers to calibrate (default none)
- int numHyperparams

  calculated number of hyperparameters augmenting the calibration parameter set, e.g., due to calibrate observation error multipliers
- RealVector invGammaAlphas

  alphas for inverse gamma distribution on hyper-params
- RealVector invGammaBetas

  alphas for inverse gamma distribution on hyper-params
- std::vector
  < Pecos::RandomVariable > invGammaDists

  distributions for hyper-params
- bool standardizedSpace

  flag indicating use of a variable transformation to standardized probability space for the model or emulator

- bool posteriorStatsKL

    flag indicating the calculation of KL divergence between prior and posterior
- bool posteriorStatsMutual

    flag indicating the calculation of mutual information between prior and posterior
- bool posteriorStatsKDE

    flag indicating the calculation of the kernel density estimate of the posteriors
- bool chainDiagnostics

    flag indicating calculation of chain diagnostics
- bool chainDiagnosticsCI

    flag indicating calculation of confidence intervals as a chain diagnositc
- bool calModelEvidence

    flag indicating calculation of the evidence of the model
- bool calModelEvidMC

    flag indicating use of Monte Carlo approximation to calculate evidence
- bool calModelEvidLaplace

    flag indicating use of Laplace approximation to calculate evidence
- int evidenceSamples

    number of samples to be used in model evidence calculation
- bool adaptPosteriorRefine

    flag indicating usage of adaptive posterior refinement; currently makes sense for unstructured grids in GP and PCE least squares/CS
- String proposalCovarType

    approach for defining proposal covariance
- RealVector proposalCovarData

    data from user input of proposal covariance
- String proposalCovarFilename

    filename for user-specified proposal covariance
- String proposalCovarInputType

    approach for defining proposal covariance
- RealMatrix acceptanceChain

    Post-processing-related controls.
- RealMatrix acceptedFnVals

    cached function values corresponding to acceptanceChain for final statistics reporting
- std::map< Real, RealVector > bestSamples

    container for managing best MCMC samples (points and associated log posterior) collected across multiple (restarted) chains
- int burnInSamples

    number of MCMC samples to discard from acceptance chain
- int subSamplingPeriod

    period or skip in post-processing the acceptance chain
- RealMatrix **chainStats**
- RealMatrix **fnStats**
- RealMatrix predVals

    Compute credibility and prediction intervals of final chain.
- RealMatrix filteredFnVals

    cached filtered function values for printing (may be a view of acceptedFnVals)
- String exportMCMCFilename

    output filename for the MCMC chain
- short exportMCMCFormat

    output formatting options for MCMC export
- short **filteredMCMCFormat**

- Real **kl_est**
- bool scaleFlag

  whether response scaling is active
- bool weightFlag

  whether weight scaling is active

Static Protected Attributes

- static NonDBayesCalibration * nonDBayesInstance

  Pointer to current class instance for use in static callback functions.

14.135.1 Detailed Description

Base class for Bayesian inference: generates posterior distribution on model parameters given experimental data.

This class will eventually provide a general-purpose framework for Bayesian inference. In the short term, it only collects shared code between QUESO and GPMSA implementations.

14.135.2 Constructor & Destructor Documentation

14.135.2.1 NonDBayesCalibration (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDBayesCalibration::adaptExpDesign, NonDBayesCalibration::adaptPosteriorRefine, Iterator::assign_rep(), Model::assign_rep(), NonDBayesCalibration::batchSize, NonDBayesCalibration::burnInSamples, NonDCalibration::calibrationData, NonDBayesCalibration::chainSamples, NonDBayesCalibration::construct_map_model(), NonDBayesCalibration::construct_mcmc_model(), Model::continuous_lower_bound(), Model::continuous_upper_bound(), Model::continuous_variables(), Dakota::copy_data_partial(), Model::cv(), NonDBayesCalibration::emulatorType, NonDCalibration::expData, Dakota::generate_system_seed(), ProblemDescDB::get_bool(), NonDBayesCalibration::hifiModel, NonDBayesCalibration::hifiSampler, NonDBayesCalibration::init_hyper_parameters(), NonDBayesCalibration::init_map_optimizer(), NonDBayesCalibration::initHifiSamples, NonDBayesCalibration::invGammaDists, Iterator::iteratedModel, NonDBayesCalibration::mapSoln, Iterator::maxEvalConcurrency, Iterator::maxIterations, NonDBayesCalibration::mcmcDerivOrder, NonDBayesCalibration::mcmcModel, Model::model_type(), Model::multivariate_distribution(), ExperimentData::num_experiments(), Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, NonDBayesCalibration::obsErrorMultiplierMode, Iterator::probDescDB, NonDBayesCalibration::randomSeed, NonDBayesCalibration::residualModel, NonDBayesCalibration::scale_model(), NonDBayesCalibration::scaleFlag, NonDBayesCalibration::standardizedSpace, NonDBayesCalibration::subSamplingPeriod, Dakota::SZ_MAX, Model::truth_model(), Analyzer::vary_pattern(), NonDBayesCalibration::weight_model(), and NonDBayesCalibration::weightFlag.

14.135.3 Member Function Documentation

14.135.3.1 void prior_mean (VectorType & *mean_vec*) const

return the mean of the prior distribution

Assume the target mean_vec is sized by client

References NonDBayesCalibration::invGammaDists, Iterator::iteratedModel, NonDBayesCalibration::mcmcModel, Model::multivariate_distribution(), Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, and NonDBayesCalibration::standardizedSpace.

14.135.3.2 void prior_variance (MatrixType & *var_mat*) const

return the covariance of the prior distribution

Assumes the target var_mat is sized by client

References NonDBayesCalibration::invGammaDists, Iterator::iteratedModel, NonDBayesCalibration::mcmcModel, Model::multivariate_distribution(), Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, and NonDBayesCalibration::standardizedSpace.

14.135.3.3 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

References NonDBayesCalibration::construct_map_optimizer(), Model::is_null(), NonDBayesCalibration::negLogPostModel, Analyzer::pre_run(), NonDBayesCalibration::residualModel, and Model::update_from_subordinate_model().

14.135.3.4 void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References NonDBayesCalibration::adaptExpDesign, NonDBayesCalibration::adaptPosteriorRefine, NonDBayesCalibration::build_model_discrepancy(), NonDBayesCalibration::calibrate(), NonDBayesCalibration::calibrate_to_hifi(), NonDBayesCalibration::calibrate_with_adaptive_emulator(), NonDBayesCalibration::calModelDiscrepancy, NonDBayesCalibration::compute_statistics(), NonDBayesCalibration::initialize_model(), NonDBayesCalibration::nonDBayesInstance, and NonDBayesCalibration::specify_prior().

14.135.3.5 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

Reimplemented in NonDGPMSABayesCalibration, NonDQUESOBayesCalibration, NonDWASABIBayesCalibration, and NonDMUQBayesCalibration.

References NonDBayesCalibration::chainDiagnostics, Model::continuous_variable_labels(), Dakota::copy_data(), Model::current_response(), NonDBayesCalibration::filteredFnVals, Response::function_labels(), Dakota::length(), NonDBayesCalibration::mcmcModel, Iterator::outputLevel, NonDBayesCalibration::posteriorStatsKL, NonDSampling::print_moments(), NonD::requestedProbLevels, and NonDBayesCalibration::residualModel.

Referenced by NonDMUQBayesCalibration::print_results(), NonDQUESOBayesCalibration::print_results(), and NonDGPMSABayesCalibration::print_results().

14.135.3.6 const Model & algorithm_space_model ( ) const [inline], [protected], [virtual]

default definition that gets redefined in selected derived Minimizers

Reimplemented from Analyzer.

References NonDBayesCalibration::mcmcModel.

14.135.3.7 void init_map_optimizer ( ) [protected]

initialize the MAP optimizer selection

Construct optimizer for MAP pre-solve Emulator: on by default; can be overridden with "pre_solve none" No emulator: off by default; can be activated with "pre_solve {sqp,nip}" relies on mapOptimizer ctor to enforce min derivative support Calculation of model evidence using Laplace approximation: this requires a MAP solve.

References Dakota::abort_handler(), NonDBayesCalibration::calModelEvidLaplace, NonDBayesCalibration::emulatorType, and NonDBayesCalibration::mapOptAlgOverride.

Referenced by NonDBayesCalibration::NonDBayesCalibration().

14.135.3.8 void map_pre_solve ( ) [protected], [virtual]

Runs a pre-solve for the MAP point. If running calibrate_to_hifi() or calibrate_with_adaptive_emulator(), propagates the solution to the mapSoln variable. Returns the optimal solution as a vector.

References Variables::continuous_variables(), Dakota::copy_data(), Model::current_variables(), Iterator::is_null(), NonDBayesCalibration::mapOptimizer, NonDBayesCalibration::mapSoln, NonDBayesCalibration::negLogPostModel, NonDBayesCalibration::print_variables(), Iterator::run(), and Iterator::variables_results().

14.135.3.9 void calibrate_with_adaptive_emulator ( ) [protected]

Run calibration, looping to refine emulator around posterior mode.

This method will perform a Bayesian calibration with an emulator, but periodically the emulator is updated with more sample points from the original model in the high-posterior-density region of parameter space.

References Dakota::abort_handler(), NonDBayesCalibration::assess_emulator_convergence(), NonDBayesCalibration::best_to_all(), NonDBayesCalibration::calibrate(), Analyzer::compactMode, Iterator::convergenceTol, NonDBayesCalibration::emulatorType, NonDBayesCalibration::filter_chain_by_conditioning(), Iterator::maxIterations, and NonDBayesCalibration::update_model().

Referenced by NonDBayesCalibration::core_run().

14.135.3.10 void build_designs (VariablesArray & *design_matrix*) [protected]

build matrix of candidate points

On entry, design_matrix already sized to numCandidates.

References Iterator::all_variables(), Iterator::assign_rep(), NonDBayesCalibration::hifiModel, NonDBayesCalibration::importCandFormat, NonDBayesCalibration::importCandPtsFile, NonDBayesCalibration::numCandidates, Iterator::outputLevel, Iterator::pre_run(), NonDBayesCalibration::randomSeed, and Analyzer::vary_pattern().

Referenced by NonDBayesCalibration::calibrate_to_hifi().

14.135.3.11 Real log_likelihood (const RealVector & *residuals,* const RealVector & *all_params*) [protected]

calculate log-likelihood from the passed residuals (assuming they are already sized and scaled by covariance / hyperparams...

Calculate the log-likelihood, accounting for contributions from covariance and hyperparameters, as well as constant term:

log(L) = -1/2∗Nr∗log(2∗pi) - 1/2∗log(det(Cov)) - 1/2∗r'(Cov^{-1})∗r

The passed residuals must already be size-adjusted, differenced with any data, if present, and scaled by covariance^{-1/2}.

References NonDCalibration::expData, Dakota::HALF_LOG_2PI, ExperimentData::half_log_cov_determinant(), Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, and NonDBayesCalibration::obsErrorMultiplierMode.

Referenced by NonDBayesCalibration::calculate_evidence(), NonDQUESOBayesCalibration::dakotaLogLikelihood(), NonDBayesCalibration::neg_log_post_resp_mapping(), and NonDDREAMBayesCalibration::sample_likelihood().

14.135.3.12 void neg_log_post_resp_mapping (const Variables & *residual_vars*, const Variables & *nlpost_vars*, const Response & *residual_resp*, Response & *nlpost_resp*) [static], [protected]

static function passed by pointer to negLogPostModel recast model

Response mapping callback used within RecastModel for MAP pre-solve. Computes

-log(post) = -log(like) - log(prior); where -log(like) = 1/2∗Nr∗log(2∗pi) + 1/2∗log(det(Cov)) + 1/2∗r'(Cov^{-1})∗r = 1/2∗Nr∗log(2∗pi) + 1/2∗log(det(Cov)) + misfit

(misfit defined as 1/2 r^T (mult^2∗Gamma_d)^{-1} r) The passed residual_resp has been differenced, interpolated, and covariance-scaled

References Response::active_set_request_vector(), NonDBayesCalibration::augment_gradient_with_log_prior(), NonDBayesCalibration::augment_hessian_with_log_prior(), ExperimentData::build_gradient_of_sum_square_residuals(), ExperimentData::build_hessian_of_sum_square_residuals(), Variables::continuous_variables(), NonDCalibration::expData, Response::function_gradient_view(), Response::function_hessian_view(), Response::function_value(), Response::function_values(), ExperimentData::half_log_cov_det_gradient(), ExperimentData::half_log_cov_det_hessian(), NonDBayesCalibration::log_likelihood(), NonDBayesCalibration::log_prior_density(), NonDBayesCalibration::nonDBayesInstance, Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, NonDBayesCalibration::obsErrorMultiplierMode, and Iterator::outputLevel.

Referenced by NonDBayesCalibration::calculate_evidence(), and NonDBayesCalibration::construct_map_model().

14.135.3.13 void scale_model ( ) [protected]

Wrap iteratedModel in a RecastModel that performs response scaling.

Wrap the residualModel in a scaling transformation, such that residualModel now contains a scaling recast model.

References Model::assign_rep(), Iterator::outputLevel, and NonDBayesCalibration::residualModel.

Referenced by NonDBayesCalibration::NonDBayesCalibration().

14.135.3.14 void weight_model ( ) [protected]

Wrap iteratedModel in a RecastModel that weights the residuals.

Setup Recast for weighting model. The weighting transformation doesn't resize, and makes no vars, active set or secondary mapping. All indices are one-to-one mapped (no change in counts).

References Dakota::abort_handler(), Model::assign_rep(), Iterator::outputLevel, Model::primary_response_fn_weights(), and NonDBayesCalibration::residualModel.

Referenced by NonDBayesCalibration::NonDBayesCalibration().

14.135.3.15 void export_chain (RealMatrix & *filtered_chain,* RealMatrix & *filtered_fn_vals*) [protected]

Print filtered posterior and function values (later: credibility and prediction intervals)

Print tabular file with filtered chain, function values, and pred values

References Variables::continuous_variables(), Variables::copy(), Model::current_response(), Model::current_variables(), NonDBayesCalibration::exportMCMCFilename, NonDBayesCalibration::exportMCMCFormat, Response::function_labels(), Model::interface_id(), NonDBayesCalibration::mcmcModel, Analyzer::numFunctions, NonDBayesCalibration::residualModel, Dakota::write_precision, and Variables::write_tabular().

14.135.4 Member Data Documentation

14.135.4.1 RealMatrix acceptanceChain [protected]

Post-processing-related controls.

accumulation of acceptance chain across restarts (stored in user-space) TO DO: retire once restarts are retired; optimize to convert to user-space only in final results

Referenced by NonDDREAMBayesCalibration::archive_acceptance_chain(), NonDGPMSABayesCalibration::cache_acceptance_chain(), NonDMUQBayesCalibration::cache_chain(), NonDDREAMBayesCalibration::cache_chain(), NonDQUESOBayesCalibration::cache_chain(), NonDBayesCalibration::calculate_kde(), NonDBayesCalibration::calibrate_to_hifi(), and NonDBayesCalibration::compute_statistics().

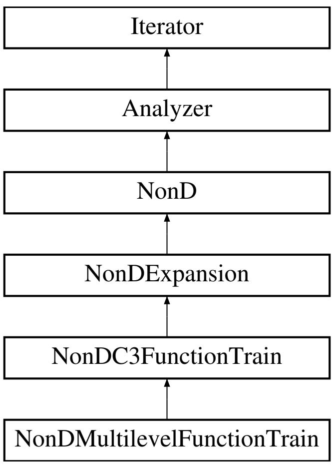
The documentation for this class was generated from the following files:

- NonDBayesCalibration.hpp
- NonDBayesCalibration.cpp

14.136 NonDC3FunctionTrain Class Reference

Nonintrusive uncertainty quantification with the C3 library ...

Inheritance diagram for NonDC3FunctionTrain:



Public Member Functions

- NonDC3FunctionTrain (ProblemDescDB &problem_db, Model &model)
  standard constructor
- ∼NonDC3FunctionTrain ()
  destructor

Protected Member Functions

- NonDC3FunctionTrain (unsigned short method_name, ProblemDescDB &problem_db, Model &model)

  base constructor for DB construction of multilevel/multifidelity PCE (method_name is not necessary, rather it is just a convenient overload allowing the derived ML FT class to bypass the standard FT ctor)
- void resolve_inputs (short &u_space_type, short &data_order)

  perform error checks and mode overrides
- void initialize_u_space_model ()

  initialize uSpaceModel polynomial approximations with PCE/SC data
- size_t collocation_points () const

  return specification for number of collocation points (may be part of a sequence specification)
- void push_increment ()

  helper function to manage different push increment cases
- void update_samples_from_order_increment ()

  update numSamplesOnModel after an order increment
- void sample_allocation_metric (Real &regress_metric, Real power)
- void print_moments (std::ostream &s)

  override certain print functions
- void print_sobol_indices (std::ostream &s)

  print global sensitivity indices
- void check_surrogate ()

  check model definition (redirect function_train model to surr-based UQ)
- void resolve_refinement ()

  assign c3AdvancementType based on user inputs for adapt_{rank,order} (fine-grained augmentation to refine{Type,Control} = uniform p-refinement)
- bool config_regression (size_t colloc_pts, size_t regress_size, int seed, Iterator &u_space_sampler, Model &g_u_model)

  configure u_space_sampler and approx_type based on regression specification
- void initialize_c3_db_options ()

  Publish options from C3 input specification (not needed if model-driven specification: already extracted by iteratedModel)
- void initialize_c3_start_rank (size_t start_rank)

  Publish configuration data for initial function train cores, prior to any adaptation.
- void initialize_c3_start_orders (const UShortArray &start_orders)

  Publish configuration data for initial function train cores, prior to any adaptation.
- void push_c3_start_rank (size_t start_rank)

  Publish configuration data for initial function train cores, prior to any adaptation.
- void push_c3_max_rank (size_t max_rank)

  Publish configuration data for initial function train cores, prior to any adaptation.
- void push_c3_start_orders (const UShortArray &start_orders)

  Publish configuration data for initial function train cores, prior to any adaptation.
- void push_c3_max_order (unsigned short max_order)

  Publish configuration data for initial function train cores, prior to any adaptation.
- void push_c3_seed (int seed)

  Publish random seed for internal C3 use.

Protected Attributes

- String importBuildPointsFile

    user-specified file for importing build points
- size_t startRankSpec

    scalar specification for initial rank (prior to adapt_rank)
- size_t maxRankSpec

    scalar specification for maximum rank (bounds adapt_rank)
- unsigned short startOrderSpec

    scalar specification for initial basis order (prior to uniform refinement)
- unsigned short maxOrderSpec

    scalar specification for maximum basis order (bounds uniform refinement)
- short c3AdvancementType

    type of advancement used by (uniform) refinement: START_{RANK,ORDER} or MAX_{RANK,ORDER,RANK_ORDER}

Private Member Functions

- size_t regression_size ()

    return the regression size used for different refinement options

Private Attributes

- size_t collocPtsSpec

    user specification for collocation_points

Additional Inherited Members

14.136.1 Detailed Description

Nonintrusive uncertainty quantification with the C3 library ...

The NonDC3FunctionTrain class uses ...

14.136.2 Constructor & Destructor Documentation

14.136.2.1 NonDC3FunctionTrain (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation using the ProblemDescDB.

References Dakota::abort_handler(), Response::active_set(), Model::assign_rep(), NonDC3FunctionTrain::check_surrogate(), NonDC3FunctionTrain::collocPtsSpec, NonDC3FunctionTrain::config_regression(), NonDExpansion::configure_expansion_orders(), NonDExpansion::construct_expansion_sampler(), Model::current_response(), NonDExpansion::dimPrefSpec, ProblemDescDB::get_bool(), ProblemDescDB::get_iv(), ProblemDescDB::get_string(), ProblemDescDB::get_ushort(), NonDC3FunctionTrain::importBuildPointsFile, NonDC3FunctionTrain::initialize_u_space_model(), Iterator::iteratedModel, Iterator::outputLevel, Iterator::probDescDB, NonDExpansion::randomSeed, NonDC3FunctionTrain::regression_size(), ActiveSet::request_values(), NonDC3FunctionTrain::resolve_inputs(), NonDC3FunctionTrain::resolve_refinement(), NonDC3FunctionTrain::startOrderSpec, and NonDExpansion::uSpaceModel.

14.136.2.2 NonDC3FunctionTrain (unsigned short *method_name*, ProblemDescDB & *problem_db*, Model & *model*) [protected]

base constructor for DB construction of multilevel/multifidelity PCE (method_name is not necessary, rather it is just a convenient overload allowing the derived ML FT class to bypass the standard FT ctor)

This constructor is called by derived class constructors.

References NonDC3FunctionTrain::check_surrogate(), and NonDC3FunctionTrain::resolve_refinement().

14.136.3 Member Function Documentation

14.136.3.1 void sample_allocation_metric (Real & *regress_metric*, Real *power*) [protected], [virtual]

```
inconvenient to recompute: store previous samples rather than
previous ranks
```

void NonDC3FunctionTrain::update_samples_from_order_decrement() { numSamplesOnModel = prevSamplesOnModel; }//requires level mgmt for persistence

Reimplemented from NonDExpansion.

References Model::approximations(), NonDC3FunctionTrain::c3AdvancementType, SharedApproxData::data_rep(), Analyzer::numFunctions, Iterator::outputLevel, Model::shared_approximation(), and NonDExpansion::uSpaceModel.

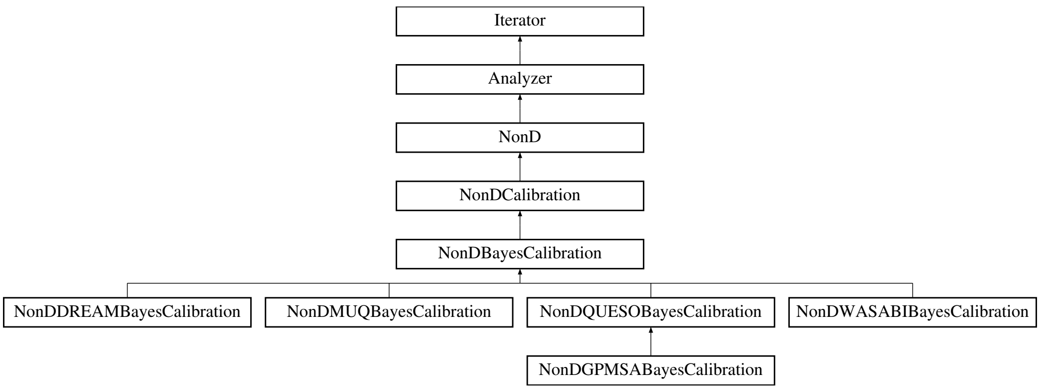
Referenced by NonDC3FunctionTrain::update_samples_from_order_increment().

The documentation for this class was generated from the following files:

- NonDC3FunctionTrain.hpp
- NonDC3FunctionTrain.cpp

14.137 NonDCalibration Class Reference

Inheritance diagram for NonDCalibration:



Public Member Functions

- NonDCalibration (ProblemDescDB &problem_db, Model &model)

  standard constructor
- ∼NonDCalibration ()

  destructor

- bool resize ()

  reinitializes iterator based on new variable size

Protected Attributes

- bool calibrationData

  flag indicating whether there is calibration data present

- ExperimentData expData

  Container for experimental data to which to calibrate model.

Additional Inherited Members

14.137.1 Detailed Description

This class ...

14.137.2 Constructor & Destructor Documentation

14.137.2.1 NonDCalibration (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References NonDCalibration::calibrationData, Model::current_variables(), NonDCalibration::expData, Iterator::iteratedModel, ExperimentData::load_data(), and Iterator::outputLevel.

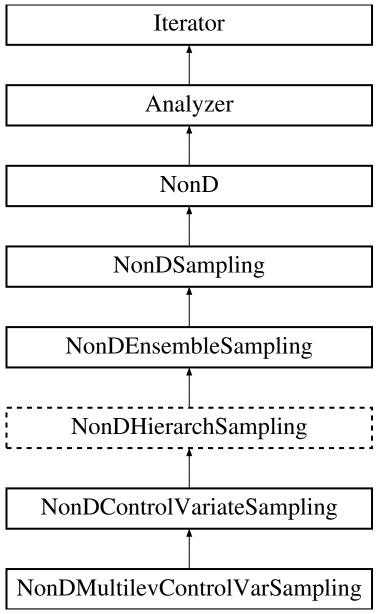
The documentation for this class was generated from the following files:

- NonDCalibration.hpp
- NonDCalibration.cpp

14.138 NonDControlVariateSampling Class Reference

Performs Multifidelity Monte Carlo sampling for UQ.

Inheritance diagram for NonDControlVariateSampling:



Public Member Functions

- NonDControlVariateSampling (ProblemDescDB &problem_db, Model &model)

    standard constructor
- ∼NonDControlVariateSampling ()

    destructor

Protected Member Functions

- void core_run ()
- void **print_variance_reduction** (std::ostream &s)
- bool lf_increment (const RealVector &eval_ratios, const SizetArray &N_lf, Real hf_target, size_t iter, size_t lev)

    perform LF sample increment as indicated by the evaluation ratio
- bool lf_increment (const Pecos::ActiveKey &lf_key, const RealVector &eval_ratios, const SizetArray &N_lf, const RealVector &hf_targets, size_t iter, size_t lev)

    perform final LF sample increment as indicated by the evaluation ratio
- void compute_mf_correlation (Real sum_L, Real sum_H, Real sum_LL, Real sum_LH, Real sum_HH, size_t N_shared, Real &var_H, Real &rho2_LH)

    compute scalar variance and correlation parameters for control variates
- void apply_mf_control (Real sum_H, Real sum_L_shared, size_t N_shared, Real sum_L_refined, size_t N_-refined, Real beta, Real &H_raw_mom)

    apply scalar control variate parameter (beta) to approximate HF moment
- void apply_mf_control (const RealMatrix &sum_H, const RealMatrix &sum_L_shared, const SizetArray &N_-shared, const RealMatrix &sum_L_refined, const SizetArray &N_refined, size_t lev, const RealVector &beta, RealVector &H_raw_mom)

    apply matrix control variate parameter (beta) to approximate HF moment

Private Member Functions

- void control_variate_mc (const Pecos::ActiveKey &active_key)

    Perform control variate Monte Carlo across two model forms, including pilot sample as online cost.

- void control_variate_mc_offline_pilot (const Pecos::ActiveKey &active_key)

  Perform control variate Monte Carlo across two model forms, segregating the pilot sample as separate offline cost.
- void control_variate_mc_pilot_projection (const Pecos::ActiveKey &active_key)

  Perform control variate Monte Carlo across two model forms, projecting estimator performance based only on the pilot sample.
- void evaluate_pilot (const Pecos::ActiveKey &active_key, Real &cost_ratio, RealVector &eval_ratios, RealVector &var_H, SizetArray &N_shared, RealVector &hf_targets, bool accumulate_cost, bool pilot_estvar)

  helper for shared code among MLCV for offline-pilot and pilot-projection
- void hf_lf_indices (size_t &hf_form_index, size_t &hf_lev_index, size_t &lf_form_index, size_t &lf_lev_index)

  define model form and resolution level indices
- void shared_increment (const Pecos::ActiveKey &agg_key, size_t iter, size_t lev)

  perform a shared increment of LF and HF samples for purposes of computing/updating the evaluation and estimator variance ratios
- bool lf_increment (size_t iter, size_t lev)

  core parameter set definition and evaluation for LF sample increment
- void compute_mf_equivalent_cost (size_t raw_N_hf, size_t raw_N_lf, Real cost_ratio)

  update equivHFEvals from HF, LF evaluation counts
- void increment_mf_equivalent_cost (size_t new_N_hf, size_t new_N_lf, Real cost_ratio)

  update equivHFEvals from HF, LF evaluation increment
- void increment_mf_equivalent_cost (size_t new_N_lf, Real cost_ratio)

  update equivHFEvals from LF evaluation increment
- void initialize_mf_sums (IntRealVectorMap &sum_L_shared, IntRealVectorMap &sum_H, IntRealVectorMap &sum_LL, IntRealVectorMap &sum_LH)

  initialize the CV accumulators for computing means, variances, and covariances across fidelity levels
- void accumulate_mf_sums (IntRealVectorMap &sum_L, SizetArray &num_L)

  update running sums for one model (sum_L) using set of model evaluations within allResponses
- void accumulate_mf_sums (IntRealVectorMap &sum_L_shared, IntRealVectorMap &sum_H, IntRealVectorMap &sum_LL, IntRealVectorMap &sum_LH, RealVector &sum_HH, SizetArray &N_shared)

  update running sums for two models from set of low/high fidelity model evaluations within allResponses
- void accumulate_mf_sums (RealVector &sum_L, RealVector &sum_H, RealVector &sum_LL, RealVector &sum_LH, RealVector &sum_HH, SizetArray &N_shared)

  update running sums for two models from set of low/high fidelity model evaluations within allResponses
- void allocate_budget (const RealVector &eval_ratios, Real cost_ratio, RealVector &hf_targets)

  scale sample profile to meeet a specified budget
- void compute_eval_ratios (const RealVector &sum_L_shared, const RealVector &sum_H, const RealVector &sum_LL, const RealVector &sum_LH, const RealVector &sum_HH, Real cost_ratio, const SizetArray &N_shared, RealVector &var_H, RealVector &rho2_LH, RealVector &eval_ratios)

  compute the LF/HF evaluation ratios across the QoI vector
- void compute_estvar_ratios (const RealVector &eval_ratios, const RealVector &rho2_LH, RealVector &estvar_ratios)

  compute ratios of MC and CVMC mean squared errors across the QoI vector
- void cv_raw_moments (IntRealVectorMap &sum_L_shared, IntRealVectorMap &sum_H, IntRealVectorMap &sum_LL, IntRealVectorMap &sum_LH, const SizetArray &N_shared, IntRealVectorMap &sum_L_refined, const SizetArray &N_refined, RealMatrix &H_raw_mom)

  compute control variate parameters for CVMC and estimate raw moments
- void apply_mf_control (const RealVector &sum_H, const RealVector &sum_L_shared, const SizetArray &N_shared, const RealVector &sum_L_refined, const SizetArray &N_refined, const RealVector &beta, RealVector &H_raw_mom)

  apply vector control variate parameter (beta) to approximate HF moment
- void update_projected_samples (const RealVector &hf_targets, const RealVector &eval_ratios, Real cost_ratio, SizetArray &N_hf, SizetArray &N_lf)

  for pilot-projection mode, update the same counts based on projections rather than accumulations

Private Attributes

- RealVector **estVarRatios**
- SizetArray **numHIter0**

Additional Inherited Members

14.138.1 Detailed Description

Performs Multifidelity Monte Carlo sampling for UQ.

Multifidelity Monte Carlo (MFMC) is a variance-reduction technique that utilitizes lower fidelity simulations that have response QoI that are correlated with the high-fidelity response QoI.

14.138.2 Constructor & Destructor Documentation

14.138.2.1 NonDControlVariateSampling (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Iterator::iteratedModel, Model::multifidelity_precedence(), and NonDEnsembleSampling::NLev.

14.138.3 Member Function Documentation

14.138.3.1 void core_run ( ) [protected], [virtual]

The primary run function manages the general case: a hierarchy of model forms (from the ordered model fidelities within a HierarchSurrModel), each of which may contain multiple discretization levels.

Reimplemented from Iterator.

Reimplemented in NonDMultilevControlVarSampling.

References Model::active_model_key(), NonDEnsembleSampling::aggregated_models_mode(), NonD::configure-_sequence(), NonDControlVariateSampling::control_variate_mc(), NonDControlVariateSampling::control_variate-_mc_offline_pilot(), NonDControlVariateSampling::control_variate_mc_pilot_projection(), Iterator::iteratedModel, NonDEnsembleSampling::numSteps, NonDEnsembleSampling::onlineCost, NonDEnsembleSampling::pilotMgmt-Mode, NonD::query_cost(), NonDEnsembleSampling::secondaryIndex, NonDEnsembleSampling::sequenceCost, NonDEnsembleSampling::sequenceType, Model::solution_level_cost_index(), Model::surrogate_model(), Dakota::-SZ_MAX, and Model::truth_model().

Referenced by NonDMultilevControlVarSampling::core_run().

14.138.3.2 bool lf_increment (const RealVector & *eval_ratios,* const SizetArray & *N_lf,* Real *hf_target,* size_t *iter,* size_t *lev*) [protected]

perform LF sample increment as indicated by the evaluation ratio

version without LF key

References NonDEnsembleSampling::average(), Analyzer::numFunctions, NonDSampling::numSamples, NonD-::one_sided_delta(), and Iterator::outputLevel.

Referenced by NonDControlVariateSampling::control_variate_mc(), NonDControlVariateSampling::control_variate-_mc_offline_pilot(), NonDControlVariateSampling::lf_increment(), NonDMultilevControlVarSampling::multilevel_-control_variate_mc_offline_pilot(), and NonDMultilevControlVarSampling::multilevel_control_variate_mc_Qcorr().

14.138.3.3 bool lf_increment (const Pecos::ActiveKey & *lf_key,* const RealVector & *eval_ratios,* const SizetArray & *N_lf,* const RealVector & *hf_targets,* size_t *iter,* size_t *lev*) [protected]

perform final LF sample increment as indicated by the evaluation ratio

version with LF key

References Model::active_model_key(), NonDEnsembleSampling::average(), Iterator::iteratedModel, NonDControlVariateSampling::lf_increment(), Analyzer::numFunctions, NonDSampling::numSamples, NonD::one_sided_delta(), Iterator::outputLevel, and NonDHierarchSampling::uncorrected_surrogate_mode().

14.138.3.4 void control_variate_mc (const Pecos::ActiveKey & *active_key*) [private]

Perform control variate Monte Carlo across two model forms, including pilot sample as online cost.

This function performs control variate MC across two combinations of model form and discretization level.

References NonDControlVariateSampling::accumulate_mf_sums(), NonDControlVariateSampling::allocate_budget(), NonDEnsembleSampling::average(), NonDEnsembleSampling::avgEstVar, NonDControlVariateSampling::compute_estvar_ratios(), NonDControlVariateSampling::compute_eval_ratios(), NonDEnsembleSampling::compute_mc_estimator_variance(), Iterator::convergenceTol, NonDEnsembleSampling::convert_moments(), NonDControlVariateSampling::cv_raw_moments(), NonDEnsembleSampling::estvar_ratios_to_avg_estvar(), NonDEnsembleSampling::estVarIter0, NonDEnsembleSampling::finalStatsType, NonDControlVariateSampling::hf_lf_indices(), NonDControlVariateSampling::increment_mf_equivalent_cost(), NonDControlVariateSampling::initialize_mf_sums(), NonDControlVariateSampling::lf_increment(), NonD::load_pilot_sample(), Iterator::maxFunctionEvals, Iterator::maxIterations, NonDEnsembleSampling::mlmfIter, NonD::momentStats, NonDEnsembleSampling::NLev, Analyzer::numFunctions, NonDSampling::numSamples, NonDEnsembleSampling::numSteps, NonD::one_sided_delta(), NonDEnsembleSampling::onlineCost, NonDEnsembleSampling::pilotSamples, NonDHierarchSampling::recover_paired_online_cost(), NonDEnsembleSampling::sequenceCost, NonDControlVariateSampling::shared_increment(), Dakota::SZ_MAX, NonDControlVariateSampling::update_projected_samples(), and NonDEnsembleSampling::varH.

Referenced by NonDControlVariateSampling::core_run().

14.138.3.5 void control_variate_mc_offline_pilot (const Pecos::ActiveKey & *active_key*) [private]

Perform control variate Monte Carlo across two model forms, segregating the pilot sample as separate offline cost.

This function performs control variate MC across two combinations of model form and discretization level.

References NonDControlVariateSampling::accumulate_mf_sums(), NonDEnsembleSampling::avgEstVar, NonDEnsembleSampling::convert_moments(), NonDControlVariateSampling::cv_raw_moments(), NonDEnsembleSampling::estvar_ratios_to_avg_estvar(), NonDControlVariateSampling::evaluate_pilot(), NonDEnsembleSampling::finalStatsType, NonDControlVariateSampling::hf_lf_indices(), NonDControlVariateSampling::increment_mf_equivalent_cost(), NonDControlVariateSampling::initialize_mf_sums(), NonDControlVariateSampling::lf_increment(), NonDEnsembleSampling::mlmfIter, NonD::momentStats, NonDEnsembleSampling::NLev, Analyzer::numFunctions, NonDSampling::numSamples, NonD::one_sided_delta(), NonDControlVariateSampling::shared_increment(), NonDControlVariateSampling::update_projected_samples(), and NonDEnsembleSampling::varH.

Referenced by NonDControlVariateSampling::core_run().

14.138.3.6 void control_variate_mc_pilot_projection (const Pecos::ActiveKey & *active_key*) [private]

Perform control variate Monte Carlo across two model forms, projecting estimator performance based only on the pilot sample.

This function performs control variate MC across two combinations of model form and discretization level.

References NonDEnsembleSampling::avgEstVar, NonDEnsembleSampling::estvar_ratios_to_avg_estvar(), NonDControlVariateSampling::evaluate_pilot(), NonDControlVariateSampling::hf_lf_indices(), NonDEnsembleSampling-

::NLev, Analyzer::numFunctions, NonDControlVariateSampling::update_projected_samples(), and NonDEnsemble-Sampling::varH.

Referenced by NonDControlVariateSampling::core_run().

14.138.3.7 bool lf_increment (size_t *iter,* size_t *lev*) [private]

core parameter set definition and evaluation for LF sample increment

shared helper

References Analyzer::evaluate_parameter_sets(), NonDEnsembleSampling::export_all_samples(), NonD-EnsembleSampling::exportSampleSets, NonDSampling::get_parameter_sets(), Iterator::iteratedModel, and Model-::surrogate_model().

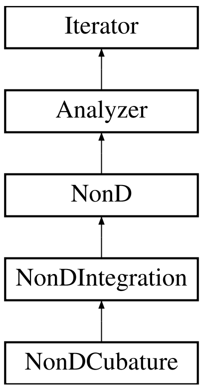
The documentation for this class was generated from the following files:

- NonDControlVariateSampling.hpp
- NonDControlVariateSampling.cpp

14.139 NonDCubature Class Reference

Derived nondeterministic class that generates N-dimensional numerical cubature points for evaluation of expectation integrals.

Inheritance diagram for NonDCubature:



Public Member Functions

- NonDCubature (Model &model, unsigned short cub_int_order)
- ∼NonDCubature ()

    destructor
- unsigned short integrand_order () const

    return cubIntOrder

Protected Member Functions

- NonDCubature (ProblemDescDB &problem_db, Model &model)

    constructor
- void initialize_grid (const std::vector< Pecos::BasisPolynomial > &poly_basis)

    initialize integration grid by drawing from polynomial basis settings

- void get_parameter_sets (Model &model)

    Generate one block of numSamples samples (ndim ∗ num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.

- void sampling_reset (size_t min_samples, bool all_data_flag, bool stats_flag)
- void increment_grid ()

    increment SSG level/TPQ order

- void increment_grid_preference (const RealVector &dim_pref)
- void increment_grid_preference ()
- void decrement_grid ()

    decrement SSG level/TPQ order

- void reset ()

    restore initial state for repeated sub-iterator executions

- size_t num_samples () const

Private Member Functions

- void assign_rule (const Pecos::MultivariateDistribution &mvd)

    define cubIntRule from random variable type

Private Attributes

- std::shared_ptr
  < Pecos::CubatureDriver > cubDriver

    convenience pointer to the numIntDriver representation

- unsigned short cubIntOrderRef

    reference point for Pecos::CubatureDriver::cubIntOrder: the original user specification for the number of Gauss points per dimension, plus any refinements posted by increment_grid()

- unsigned short cubIntRule

    the isotropic cubature integration rule

Additional Inherited Members

14.139.1 Detailed Description

Derived nondeterministic class that generates N-dimensional numerical cubature points for evaluation of expectation integrals.

This class is used by NonDPolynomialChaos, but could also be used for general numerical integration of moments. It employs Stroud cubature rules and extensions by D. Xiu.

14.139.2 Constructor & Destructor Documentation

14.139.2.1 NonDCubature (Model & *model,* unsigned short *cub_int_order*)

This alternate constructor is used for on-the-fly generation and evaluation of numerical cubature points.

References NonDCubature::assign_rule(), NonDCubature::cubDriver, NonDCubature::cubIntOrderRef, Model::multivariate_distribution(), and NonDIntegration::numIntDriver.

14.139.2.2 NonDCubature (ProblemDescDB & *problem_db,* Model & *model*) [protected]

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification. It is not currently used, as there is not yet a separate nond_cubature method specification.

References NonDCubature::assign_rule(), NonDCubature::cubDriver, NonDCubature::cubIntOrderRef, NonDCubature::cubIntRule, Iterator::maxEvalConcurrency, Model::multivariate_distribution(), and NonDIntegration::numIntDriver.

14.139.3 Member Function Documentation

14.139.3.1 void sampling_reset (size_t *min_samples,* bool *all_data_flag,* bool *stats_flag*) [protected], [virtual]

used by DataFitSurrModel::build_global() to publish the minimum number of points needed from the cubature routine in order to build a particular global approximation.

Reimplemented from Iterator.

References NonDCubature::cubDriver.

14.139.3.2 void increment_grid_preference (const RealVector & *dim_pref*) [inline], [protected], [virtual]

Should not be used, but one of virtual function pair must be defined.

Reimplemented from NonDIntegration.

References NonDCubature::increment_grid().

14.139.3.3 void increment_grid_preference ( ) [inline], [protected], [virtual]

Should not be used, but one of virtual function pair must be defined.

Reimplemented from NonDIntegration.

References NonDCubature::increment_grid().

14.139.3.4 size_t num_samples ( ) const [inline], [protected], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.

References NonDCubature::cubDriver.

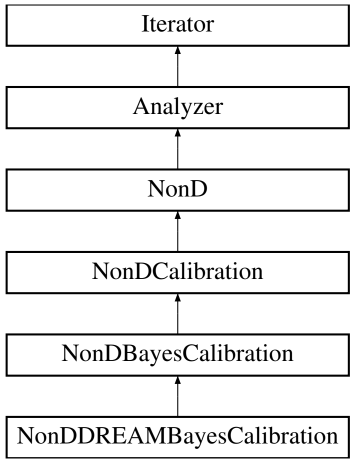
The documentation for this class was generated from the following files:

- NonDCubature.hpp
- NonDCubature.cpp

14.140 NonDDREAMBayesCalibration Class Reference

Bayesian inference using the DREAM approach.

Inheritance diagram for NonDDREAMBayesCalibration:



Public Member Functions

- NonDDREAMBayesCalibration (ProblemDescDB &problem_db, Model &model)

    standard constructor
- ∼NonDDREAMBayesCalibration ()

    destructor

Static Public Member Functions

- static void problem_size (int &chain_num, int &cr_num, int &gen_num, int &pair_num, int &par_num)

    initializer for problem size characteristics in DREAM
- static void problem_value (std::string ∗chain_filename, std::string ∗gr_filename, double &gr_threshold, int &jumpstep, double limits[ ], int par_num, int &printstep, std::string ∗restart_read_filename, std::string ∗restart-_write_filename)

    Filename and data initializer for DREAM.
- static double prior_density (int par_num, double zp[ ])

    Compute the prior density at specified point zp.
- static double ∗ prior_sample (int par_num)

    Sample the prior and return an array of parameter values.
- static double sample_likelihood (int par_num, double zp[ ])

    Likelihood function for call-back from DREAM to DAKOTA for evaluation.

Protected Member Functions

- void calibrate ()
- void archive_acceptance_chain ()

    save the final x-space acceptance chain and corresponding function values

Static Protected Member Functions

- static void cache_chain (const double ∗const z)

    Callback to archive the chain from DREAM, potentially leaving it in u-space.

Protected Attributes

- RealVector paramMins

  lower bounds on calibrated parameters
- RealVector paramMaxs

  upper bounds on calibrated parameters
- int numChains

  number of concurrent chains
- int numGenerations

  number of generations
- int numCR

  number of CR-factors
- int crossoverChainPairs

  number of crossover chain pairs
- Real grThreshold

  threshold for the Gelmin-Rubin statistic
- int jumpStep

  how often to perform a long jump in generations
- boost::mt19937 rnumGenerator

  random number engine for sampling the prior

Static Private Attributes

- static NonDDREAMBayesCalibration ∗ nonDDREAMInstance

  Pointer to current class instance for use in static callback functions.

Additional Inherited Members

14.140.1 Detailed Description

Bayesian inference using the DREAM approach.

This class performed Bayesian calibration using the DREAM (Markov Chain Monte Carlo acceleration by Differential Evolution) implementation of John Burkhardt (FSU), adapted from that of Guannan Zhang (ORNL)

14.140.2 Constructor & Destructor Documentation

14.140.2.1 NonDDREAMBayesCalibration (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References NonDBayesCalibration::chainSamples, NonDDREAMBayesCalibration::crossoverChainPairs, NonDDREAMBayesCalibration::grThreshold, NonDDREAMBayesCalibration::jumpStep, NonDDREAMBayesCalibration::numChains, NonDDREAMBayesCalibration::numCR, and NonDDREAMBayesCalibration::numGenerations.

14.140.3 Member Function Documentation

14.140.3.1 void problem_size (int & *chain_num,* int & *cr_num,* int & *gen_num,* int & *pair_num,* int & *par_num*) [static]

initializer for problem size characteristics in DREAM

See documentation in DREAM examples)

References NonDDREAMBayesCalibration::crossoverChainPairs, NonDDREAMBayesCalibration::nonDDREAMInstance, NonDDREAMBayesCalibration::numChains, Analyzer::numContinuousVars, NonDDREAMBayesCalibration::numCR, NonDDREAMBayesCalibration::numGenerations, and NonDBayesCalibration::numHyperparams.

14.140.3.2 void problem_value (std::string ∗ *chain_filename,* std::string ∗ *gr_filename,* double & *gr_threshold,* int & *jumpstep,* double *limits[],* int *par_num,* int & *printstep,* std::string ∗ *restart_read_filename,* std::string ∗ *restart_write_filename*) [static]

Filename and data initializer for DREAM.

See documentation in DREAM examples)

References NonDDREAMBayesCalibration::grThreshold, NonDDREAMBayesCalibration::jumpStep, NonDDREAMBayesCalibration::nonDDREAMInstance, NonDDREAMBayesCalibration::numChains, NonDDREAMBayesCalibration::paramMaxs, and NonDDREAMBayesCalibration::paramMins.

14.140.3.3 double prior_density (int *par_num,* double *zp[]*) [static]

Compute the prior density at specified point zp.

See documentation in DREAM examples

References NonDBayesCalibration::nonDBayesInstance, and NonDBayesCalibration::prior_density().

14.140.3.4 double ∗ prior_sample (int *par_num*) [static]

Sample the prior and return an array of parameter values.

See documentation in DREAM examples

References NonDBayesCalibration::nonDBayesInstance, NonDDREAMBayesCalibration::nonDDREAMInstance, and NonDDREAMBayesCalibration::rnumGenerator.

14.140.3.5 double sample_likelihood (int *par_num,* double *zp[]*) [static]

Likelihood function for call-back from DREAM to DAKOTA for evaluation.

Static callback function to evaluate the likelihood

References Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_values(), NonDBayesCalibration::log_likelihood(), NonDDREAMBayesCalibration::nonDDREAMInstance, Iterator::outputLevel, and NonDBayesCalibration::residualModel.

14.140.3.6 void calibrate ( ) [protected], [virtual]

Perform the uncertainty quantification DREAM will callback to cache_chain to store the chain

Implements NonDBayesCalibration.

References Dakota::abort_handler(), NonDDREAMBayesCalibration::archive_acceptance_chain(), NonDDREAMBayesCalibration::cache_chain(), NonDCalibration::calibrationData, NonDBayesCalibration::chainSamples, NonDBayesCalibration::compute_statistics(), Model::continuous_variables(), NonDBayesCalibration::initialize_model(), NonDBayesCalibration::mcmcModel, Model::multivariate_distribution(), NonDDREAMBayesCalibration::nonDDREAMInstance, Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, NonDBayesCalibration::obsErrorMultiplierMode, NonDDREAMBayesCalibration::paramMaxs, NonDDREAMBayesCalibration::paramMins, NonDBayesCalibration::randomSeed, NonDDREAMBayesCalibration::rnumGenerator, and NonDBayesCalibration::standardizedSpace.

14.140.3.7 void cache_chain (const double *const z) [static], [protected]

Callback to archive the chain from DREAM, potentially leaving it in u-space.

Archive the chain from DREAM. This default implementation is aggregating from the parallel chains in a round-robin fashion.

References NonDBayesCalibration::acceptanceChain, NonDDREAMBayesCalibration::nonDDREAMInstance, Analyzer::num_samples(), NonDDREAMBayesCalibration::numChains, Analyzer::numContinuousVars, NonDDREAMBayesCalibration::numGenerations, and NonDBayesCalibration::numHyperparams.

Referenced by NonDDREAMBayesCalibration::calibrate().

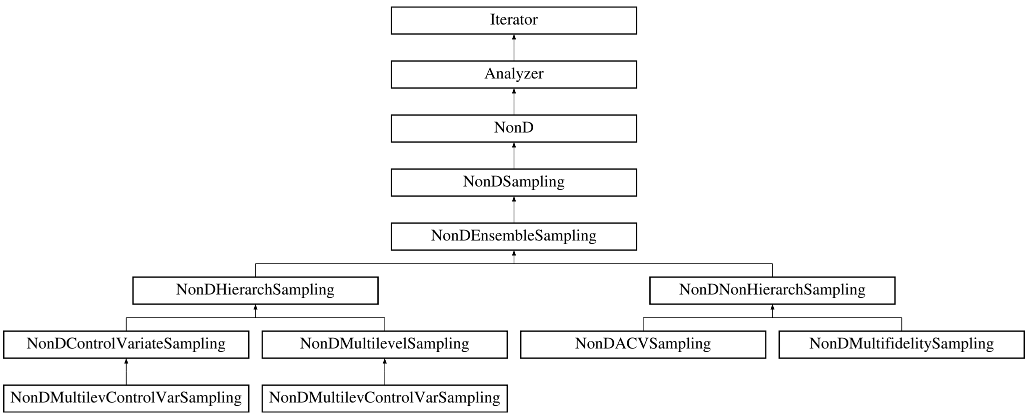
The documentation for this class was generated from the following files:

- NonDDREAMBayesCalibration.hpp
- NonDDREAMBayesCalibration.cpp

14.141 NonDEnsembleSampling Class Reference

Base class for Monte Carlo sampling across Model ensembles.

Inheritance diagram for NonDEnsembleSampling:



Public Member Functions

- NonDEnsembleSampling (ProblemDescDB &problem_db, Model &model)

    standard constructor

- ∼NonDEnsembleSampling ()

    destructor (virtual declaration should be redundant with ∼Iterator, but this is top of MLMF diamond so doesn't hurt to be explicit)

- bool resize ()

    reinitializes iterator based on new variable size

Protected Member Functions

- virtual void **print_variance_reduction** (std::ostream &s)
- void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void post_run (std::ostream &s)

  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final iterator results
- void initialize_final_statistics ()

  initializes finalStatistics for storing NonD final results
- void update_final_statistics ()

  update finalStatistics::functionValues
- bool seed_updated ()
- void active_set_mapping ()

  in the case of sub-iteration, map from finalStatistics.active_set() requests to activeSet used in evaluate_parameter_-sets()
- void aggregated_models_mode ()

  synchronize iteratedModel and activeSet on AGGREGATED_MODELS mode
- void bypass_surrogate_mode ()

  synchronize iteratedModel and activeSet on BYPASS_SURROGATE mode
- void assign_specification_sequence (size_t index)

  advance any sequence specifications
- int seed_sequence (size_t index)

  extract current random seed from randomSeedSeqSpec
- void increment_samples (SizetArray &N_l, size_t num_samples)

  increment samples array with a shared scalar
- void compute_mc_estimator_variance (const RealVector &var_l, const SizetArray &N_l, RealVector &mc_-est_var)

  compute the variance of the mean estimator (Monte Carlo sample average)
- void project_mc_estimator_variance (const RealVector &var_l, const SizetArray &N_l, size_t new_samp, RealVector &mc_est_var)

  compute the variance of the mean estimator (Monte Carlo sample average) after projection with additional samples (var_l remains fixed)
- void estvar_ratios_to_avg_estvar (const RealVector &estvar_ratios, const RealVector &var_H, const Sizet-Array &N_H, Real &avg_est_var)

  convert estimator variance ratios to average estimator variance
- void compute_mf_control (Real sum_L, Real sum_H, Real sum_LL, Real sum_LH, size_t N_shared, Real &beta)

  compute scalar control variate parameters
- void compute_mf_control (const RealMatrix &sum_L, const RealMatrix &sum_H, const RealMatrix &sum_LL, const RealMatrix &sum_LH, const SizetArray &N_shared, size_t lev, RealVector &beta)

  compute matrix control variate parameters
- void compute_mf_control (const RealVector &sum_L, const RealVector &sum_H, const RealVector &sum_LL, const RealVector &sum_LH, const SizetArray &N_shared, RealVector &beta)

  compute vector control variate parameters
- void export_all_samples (String root_prepend, const Model &model, size_t iter, size_t step)

  export allSamples to tagged tabular file
- void convert_moments (const RealMatrix &raw_mom, RealMatrix &final_mom)

  convert uncentered raw moments (multilevel expectations) to standardized moments
- Real sum (const Real ∗vec, size_t vec_len) const

compute sum of a set of observations
- Real average (const Real ∗vec, size_t vec_len) const

  compute average of a set of observations
- Real average (const RealVector &vec) const

  compute average of a set of observations
- Real average (const SizetArray &sa) const

  compute average of a set of observations
- void average (const RealMatrix &mat, size_t avg_index, RealVector &avg_vec) const

  compute row-averages for each column or column-averages for each row

Static Protected Member Functions

- static void uncentered_to_centered (Real rm1, Real rm2, Real rm3, Real rm4, Real &cm1, Real &cm2, Real &cm3, Real &cm4, size_t Nlq)

  convert uncentered (raw) moments to centered moments; biased estimators
- static void uncentered_to_centered (Real rm1, Real rm2, Real rm3, Real rm4, Real &cm1, Real &cm2, Real &cm3, Real &cm4)

  convert uncentered (raw) moments to centered moments; unbiased estimators
- static void centered_to_standard (Real cm1, Real cm2, Real cm3, Real cm4, Real &sm1, Real &sm2, Real &sm3, Real &sm4)

  convert centered moments to standardized moments
- static void check_negative (Real &cm)

  detect, warn, and repair a negative central moment (for even orders)

Protected Attributes

- size_t numSteps

  number of model forms/resolution in the (outer) sequence
- short sequenceType

  type of model sequence enumerated with primary MF/ACV loop over steps
- size_t secondaryIndex

  setting for the inactive model dimension not traversed by primary MF/ACV loop over steps
- RealVector sequenceCost

  relative costs of model forms/resolution levels within a 1D sequence
- Sizet3DArray NLev

  total number of successful sample evaluations (excluding faults) for each model form, discretization level, and QoI
- SizetArray pilotSamples

  store the pilot_samples input specification, prior to run-time invocation of load_pilot_sample()
- short pilotMgmtMode

  enumeration for pilot management modes: ONLINE_PILOT (default), OFFLINE_PILOT, PILOT_PROJECTION
- bool onlineCost

  indicates use of online cost recovery rather than offline user-specified cost ratios
- SizetSizetPairArray costMetadataIndices

  indices of cost data within response metadata, one per model form
- SizetArray randomSeedSeqSpec

  user specification for seed_sequence
- size_t mlmfIter

  major iteration counter
- Real avgEstVar

  final estimator variance for targeted moment (usually mean), averaged across QoI
- Real equivHFEvals

equivalent number of high fidelity evaluations accumulated using samples across multiple model forms and/or discretization levels

- RealVector varH

  variances for HF truth (length numFunctions)

- RealVector estVarIter0

  initial estimator variance from shared pilot (no CV reduction)

- short finalStatsType

  QOI_STATISTICS (moments, level mappings) or ESTIMATOR_PERFORMANCE (for model tuning of estVar,equivHFEvals by an outer loop)

- bool exportSampleSets

  if defined, export each of the sample increments in ML, CV, MLCV using tagged tabular files

- unsigned short exportSamplesFormat

  format for exporting sample increments using tagged tabular files

Private Attributes

- size_t seedIndex

  cache state of seed sequence for use in seed_updated()

Additional Inherited Members

14.141.1 Detailed Description

Base class for Monte Carlo sampling across Model ensembles.

Monte Carlo methods may employ model ensembles as variance-reduction techniques, utilitizing lower fidelity simulations that have response QoI that are correlated with the high-fidelity response QoI.

14.141.2 Constructor & Destructor Documentation

14.141.2.1 NonDEnsembleSampling (ProblemDescDB & *problem_db*, Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDEnsembleSampling::initialize_final_statistics(), Iterator::maxFunctionEvals, Iterator::maxIterations, NonDEnsembleSampling::pilotMgmtMode, NonDSampling::sampleType, and Dakota::SZ_MAX.

14.141.3 Member Function Documentation

14.141.3.1 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

Reimplemented in NonDNonHierarchSampling, and NonDMultilevControlVarSampling.

References Model::clear_model_keys(), NonDEnsembleSampling::equivHFEvals, Iterator::iteratedModel, NonD-EnsembleSampling::mlmfIter, NonDSampling::numLHSRuns, NonDSampling::pre_run(), NonDSampling::random-Seed, NonDEnsembleSampling::seed_sequence(), and NonDSampling::seedSpec.

Referenced by NonDMultilevControlVarSampling::pre_run(), and NonDNonHierarchSampling::pre_run().

14.141.3.2 void post_run (std::ostream & *s*) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Analyzer.

References Analyzer::post_run(), and NonDEnsembleSampling::update_final_statistics().

14.141.3.3 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

References NonD::archive_equiv_hf_evals(), NonDSampling::archive_moments(), NonDEnsembleSampling-::equivHFEvals, Iterator::iteratedModel, NonDEnsembleSampling::NLev, NonDEnsembleSampling::pilotMgmt-Mode, NonDSampling::print_moments(), NonD::print_multilevel_evaluation_summary(), Model::response_labels(), NonDSampling::statsFlag, Model::truth_model(), and Dakota::write_precision.

14.141.3.4 void initialize_final_statistics ( ) [protected], [virtual]

initializes finalStatistics for storing NonD final results

Default definition of virtual function (used by sampling, reliability, and stochastic expansion methods) defines the set of statistical results to include the first two moments and level mappings for each QoI.

Reimplemented from NonD.

References ActiveSet::derivative_vector(), NonD::finalStatistics, NonDEnsembleSampling::finalStatsType, Response::function_labels(), Model::inactive_continuous_variable_ids(), NonD::initialize_final_statistics(), and Iterator::iteratedModel.

Referenced by NonDEnsembleSampling::NonDEnsembleSampling().

14.141.3.5 bool seed_updated ( ) [inline], [protected], [virtual]

extract an active seed from a seed sequence

Reimplemented from NonDSampling.

References NonDEnsembleSampling::seedIndex, and Dakota::SZ_MAX.

14.141.3.6 void active_set_mapping ( ) [protected], [virtual]

in the case of sub-iteration, map from finalStatistics.active_set() requests to activeSet used in evaluate_parameter-_sets()

Map ASV/DVV requests in final statistics into activeSet for use in evaluate_parameter_sets()

Reimplemented from NonDSampling.

References NonDSampling::active_set_mapping(), Iterator::activeSet, NonDEnsembleSampling::finalStatsType, and ActiveSet::request_values().

14.141.3.7 int seed_sequence (size_t *index*) [inline], [protected]

extract current random seed from randomSeedSeqSpec

extract an active seed from a seed sequence

References NonDEnsembleSampling::mlmfIter, NonDEnsembleSampling::randomSeedSeqSpec, NonDEnsembleSampling::seedIndex, Dakota::SZ_MAX, and NonDSampling::varyPattern.

Referenced by NonDEnsembleSampling::assign_specification_sequence(), and NonDEnsembleSampling::pre_run().

14.141.3.8 void uncentered_to_centered (Real *rm1,* Real *rm2,* Real *rm3,* Real *rm4,* Real & *cm1,* Real & *cm2,* Real & *cm3,* Real & *cm4,* size_t *Nlq*) [inline], [static], [protected]

convert uncentered (raw) moments to centered moments; biased estimators

For single-level moment calculations with a scalar Nlq.

Referenced by NonDEnsembleSampling::convert_moments().

14.141.3.9 void uncentered_to_centered (Real *rm1,* Real *rm2,* Real *rm3,* Real *rm4,* Real & *cm1,* Real & *cm2,* Real & *cm3,* Real & *cm4*) [inline], [static], [protected]

convert uncentered (raw) moments to centered moments; unbiased estimators

For single-level moment calculations with a scalar Nlq.

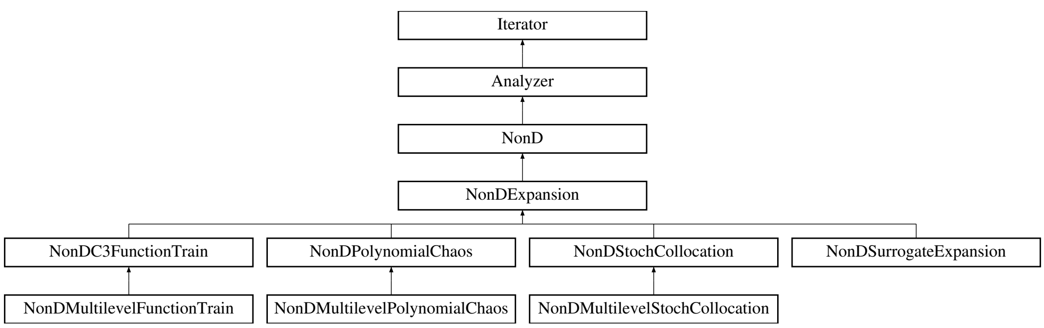
The documentation for this class was generated from the following files:

- NonDEnsembleSampling.hpp
- NonDEnsembleSampling.cpp

14.142 NonDExpansion Class Reference

Base class for polynomial chaos expansions (PCE), stochastic collocation (SC) and functional tensor train (FT)

Inheritance diagram for NonDExpansion:



Public Member Functions

- NonDExpansion (ProblemDescDB &problem_db, Model &model)

    standard constructor
- NonDExpansion (unsigned short method_name, Model &model, short exp_coeffs_approach, const RealVector &dim_pref, int seed, short refine_type, short refine_control, short covar_control, Real colloc_ratio, short rule_nest, short rule_growth, bool piecewise_basis, bool use_derivs)

    alternate constructor
- ∼NonDExpansion ()

    destructor
- bool resize ()

    reinitializes iterator based on new variable size
- void derived_init_communicators (ParLevLIter pl_iter)

    derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

    derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

    derived class contributions to freeing the communicators associated with this Iterator instance
- void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

    set primaryA{CV,DIV,DRV}MapIndices, secondaryA{CV,DIV,DRV}MapTargets within derived Iterators; supports computation of higher-level sensitivities in nested contexts (e.g., derivatives of statistics w.r.t. inserted design variables)
- void core_run ()

    perform a forward uncertainty propagation using PCE/SC methods
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

    print the final statistics
- const Model & algorithm_space_model () const
- virtual size_t collocation_points () const

    return specification for number of collocation points (may be part of a sequence specification)
- virtual int random_seed () const

    return specification for random seed (may be part of a sequence specification)
- virtual int first_seed () const

    return first seed in sequence specification (defaults to random_seed())
- virtual void select_refinement_points (const RealVectorArray &candidate_samples, unsigned short batch_size, RealMatrix &best_samples)

    evaluate allSamples for inclusion in the (PCE regression) approximation and retain the best set (well spaced) of size batch_size
- virtual void append_expansion ()

    generate numSamplesOnModel, append to approximation data, and update QoI expansions
- virtual void append_expansion (const RealMatrix &samples, const IntResponseMap &resp_map)

    append new data to uSpaceModel and, when appropriate, update expansion order
- virtual void assign_discrepancy_mode ()

    verify supported and define default discrepancy emulation mode
- virtual void assign_hierarchical_response_mode ()

    define the surrogate response mode for a hierarchical model in multilevel/multifidelity expansions
- virtual void infer_pilot_sample (size_t num_steps, SizetArray &delta_N_l)
- size_t maximum_refinement_iterations () const

    return maxRefineIterations
- void maximum_refinement_iterations (size_t max_refine_iter)

    set maxRefineIterations

Protected Member Functions

- virtual void resolve_inputs (short &u_space_type, short &data_order)

  perform error checks and mode overrides
- virtual void initialize_u_space_model ()

  initialize uSpaceModel polynomial approximations with PCE/SC data
- virtual void initialize_expansion ()

  initialize random variable definitions and final stats arrays
- virtual void compute_expansion ()

  form the expansion by calling uSpaceModel.build_approximation()
- virtual void finalize_expansion ()

  finalize mappings for the uSpaceModel
- virtual void assign_specification_sequence ()

  assign the current values from the input specification sequence
- virtual void increment_specification_sequence ()

  increment the input specification sequence and assign values
- virtual void update_expansion ()

  update an expansion; avoids overhead in compute_expansion()
- virtual void combined_to_active ()

  combine coefficients, promote to active, and update statsMetricMode
- virtual void archive_coefficients ()

  archive expansion coefficients, as supported by derived instance
- virtual void push_increment ()

  helper function to manage different push increment cases
- virtual void pop_increment ()

  helper function to manage different pop increment cases
- virtual Real compute_covariance_metric (bool revert, bool print_metric)

  compute 2-norm of change in response covariance
- virtual Real compute_level_mappings_metric (bool revert, bool print_metric)

  compute 2-norm of change in final statistics
- virtual void compute_statistics (short results_state=FINAL_RESULTS)

  calculate analytic and numerical statistics from the expansion, supporting {REFINEMENT,INTERMEDIATE,FINAL}_-RESULTS modes
- virtual void pull_candidate (RealVector &stats_star)

  extract statistics from native stats arrays for a selected candidate
- virtual void push_candidate (const RealVector &stats_star)

  restore statistics into native stats arrays for a selected candidate
- virtual void initialize_ml_regression (size_t num_lev, bool &import_pilot)

  initializations for multilevel_regression()
- virtual void increment_sample_sequence (size_t new_samp, size_t total_samp, size_t step)

  increment sequence in numSamplesOnModel for multilevel_regression()
- virtual void sample_allocation_metric (Real &metric, Real power)

  accumulate one of the level metrics for {RIP,RANK}_SAMPLING cases
- virtual void compute_sample_increment (const RealVector &lev_metrics, const SizetArray &N_l, SizetArray &delta_N_l)

  compute delta_N_l for {RIP,RANK}_SAMPLING cases
- virtual void finalize_ml_regression ()

  finalizations for multilevel_regression()
- virtual void update_samples_from_order_increment ()

  update numSamplesOnModel after an order increment
- virtual void update_samples_from_order_decrement ()

update (restore previous) numSamplesOnModel after an order decrement

- virtual void print_sobol_indices (std::ostream &s)

  print global sensitivity indices
- void initialize_response_covariance ()

  set covarianceControl defaults and shape respCovariance
- void update_final_statistics ()

  update function values within finalStatistics
- void update_final_statistics_gradients ()

  update function gradients within finalStatistics
- void initialize_u_space_grid ()

  helper for initializing a numerical integration grid
- void check_dimension_preference (const RealVector &dim_pref) const

  check length and content of dimension preference vector
- void construct_cubature (Iterator &u_space_sampler, Model &g_u_model, unsigned short cub_int_order)

  assign a NonDCubature instance within u_space_sampler
- void construct_quadrature (Iterator &u_space_sampler, Model &g_u_model, unsigned short quad_order, const RealVector &dim_pref)

  assign a NonDQuadrature instance within u_space_sampler based on a quad_order specification
- void construct_quadrature (Iterator &u_space_sampler, Model &g_u_model, unsigned short quad_order, const RealVector &dim_pref, int filtered_samples)

  assign a NonDQuadrature instance within u_space_sampler that generates a filtered tensor product sample set
- void construct_quadrature (Iterator &u_space_sampler, Model &g_u_model, unsigned short quad_order, const RealVector &dim_pref, int random_samples, int seed)

  assign a NonDQuadrature instance within u_space_sampler that samples randomly from a tensor product multi-index
- void construct_sparse_grid (Iterator &u_space_sampler, Model &g_u_model, unsigned short ssg_level, const RealVector &dim_pref)

  assign a NonDSparseGrid instance within u_space_sampler
- void configure_expansion_orders (unsigned short exp_order, const RealVector &dim_pref, UShortArray &exp_orders)

  configure exp_orders from inputs
- void configure_pecos_options ()

  configure expansion and basis configuration options for Pecos polynomial approximations
- void construct_expansion_sampler (unsigned short sample_type, const String &rng, unsigned short integration_refine=NO_INT_REFINE, const IntVector &refine_samples=IntVector(), const String &import_approx_file=String(), unsigned short import_approx_format=TABULAR_ANNOTATED, bool import_approx_active_only=false)

  construct the expansionSampler for evaluating samples on uSpaceModel
- void multifidelity_expansion ()

  construct a multifidelity expansion, across model forms or discretization levels
- void multilevel_regression ()

  allocate a multilevel expansion based on some approximation to an optimal resource allocation across model forms/discretization levels
- void configure_indices (size_t group, size_t form, size_t lev, short seq_type)

  configure response mode and active/truth/surrogate model keys within a hierarchical model. seq_type is the type of sequence that defines the active dimension for traversing a model sequence.
- Real sequence_cost (size_t step, const RealVector &cost)

  return aggregate cost (one or more models) for a level sample
- void compute_equivalent_cost (const SizetArray &N_l, const RealVector &cost)

  compute equivHFEvals from samples per level and cost per evaluation
- void compute_sample_increment (const RealVector &agg_var, const RealVector &cost, Real sum_root_var_cost, Real eps_sq_div_2, const SizetArray &N_l, SizetArray &delta_N_l)

  compute increment in samples for multilevel_regression() based on ESTIMATOR_VARIANCE

- size_t collocation_points (size_t index) const
  return number of collocation points for index within model sequence
- int seed_sequence (size_t index) const
  return random seed for index within model sequence
- void refine_expansion ()
  refine the reference expansion found by compute_expansion() using uniform/adaptive p-/h-refinement strategies
- void pre_refinement ()
  initialization of expansion refinement, if necessary
- size_t core_refinement (Real &metric, bool revert=false, bool print_metric=true)
  advance the refinement strategy one step
- void post_refinement (Real &metric, bool reverted=false)
  finalization of expansion refinement, if necessary
- void increment_grid (bool update_anisotropy=true)
  helper function to manage different grid increment cases
- void decrement_grid ()
  helper function to manage different grid decrement cases
- void merge_grid ()
  helper function to manage different grid merge cases
- void increment_order_and_grid ()
  uniformly increment the expansion order and structured/unstructured grid (PCE and FT)
- void decrement_order_and_grid ()
  uniformly decrement the expansion order and structured/unstructured grid (PCE and FT)
- void update_model_from_samples ()
  publish numSamplesOnModel update to the DataFitSurrModel instance
- void update_u_space_sampler (size_t sequence_index, const UShortArray &approx_orders)
  perform sampler updates after a change to numSamplesOnModel (shared code from ML/MF updaters)
- void refinement_statistics_mode (short stats_mode)
  update statsMetricMode, here and in Pecos::ExpansionConfigOptions
- void metric_roll_up (short results_state=FINAL_RESULTS)
  perform any required expansion roll-ups prior to metric computation
- void aggregate_variance (Real &agg_var_l)
  Aggregate variance across the set of QoI for a particular model level.
- void compute_covariance ()
  calculate the response covariance (diagonal or full matrix) for the expansion indicated by statsMetricMode
- void compute_active_covariance ()
  calculate the response covariance of the active expansion
- void compute_combined_covariance ()
  calculate the response covariance of the combined expansion
- void compute_active_diagonal_variance ()
  calculate the diagonal response variance of the active expansion
- void compute_combined_diagonal_variance ()
  calculate the diagonal response variance of the cmbined expansion
- void compute_off_diagonal_covariance ()
  calculate off diagonal terms in respCovariance(i,j) for j<i for the expansion indicated by statsMetricMode
- void compute_active_off_diagonal_covariance ()
  calculate off diagonal terms in respCovariance(i,j) for j<i using the active expansion coefficients
- void compute_combined_off_diagonal_covariance ()
  calculate off diagonal terms in respCovariance(i,j) for j<i using the combined expansion coefficients
- void compute_moments ()
  compute expansion moments; this uses a lightweight approach for incremental statistics (no additional moments; no finalStatistics update)

- void compute_level_mappings ()

  compute all analytic/numerical level mappings; this uses a lightweight approach for incremental statistics (no derivatives, no finalStatistics update)
- void compute_numerical_level_mappings ()

  compute only numerical level mappings; this uses a lightweight approach for incremental statistics (no derivatives, no finalStatistics update)
- void compute_sobol_indices ()

  compute Sobol' indices for main, interaction, and total effects; this is intended for incremental statistics
- void print_covariance (std::ostream &s)

  print resp{Variance,Covariance}
- void print_variance (std::ostream &s, const RealVector &resp_var, const String &prepend="")

  print resp_var (response variance vector) using optional pre-pend
- void print_covariance (std::ostream &s, const RealSymMatrix &resp_covar, const String &prepend="")

  print resp_covar (response covariance matrix) using optional pre-pend
- void archive_moments ()

  archive the central moments (numerical and expansion) to ResultsDB
- void archive_sobol_indices ()

  archive the Sobol' indices to the resultsDB
- void **pull_reference** (RealVector &stats_ref)
- void **push_reference** (const RealVector &stats_ref)
- void pull_lower_triangle (const RealSymMatrix &mat, RealVector &vec, size_t offset=0)

  pull lower triangle of symmetric matrix into vector
- void push_lower_triangle (const RealVector &vec, RealSymMatrix &mat, size_t offset=0)

  push vector into lower triangle of symmetric matrix
- int terms_ratio_to_samples (size_t num_exp_terms, Real colloc_ratio)

  convert number of regression terms and collocation ratio to a number of collocation samples
- Real terms_samples_to_ratio (size_t num_exp_terms, int samples)

  convert number of regression terms and number of collocation samples to a collocation ratio

Protected Attributes

- Model uSpaceModel

  Model representing the approximate response function in u-space, after u-space recasting and polynomial data fit recursions.
- Iterator expansionSampler

  Iterator used for sampling on the uSpaceModel to generate approximate probability/reliability/response level statistics. Currently this is an LHS sampling instance, but AIS could also be used.
- Iterator importanceSampler

  Iterator used to refine the approximate probability estimates generated by the expansionSampler using importance sampling.
- short expansionCoeffsApproach

  method for collocation point generation and subsequent calculation of the expansion coefficients
- short expansionBasisType

  type of expansion basis: DEFAULT_BASIS or Pecos::{NODAL,HIERARCHICAL}_INTERPOLANT for SC or Pecos::{TENSOR_PRODUCT,TOTAL_ORDER,ADAPTED}_BASIS for PCE regression
- short statsMetricMode

  type of statistical metric roll-up: {NO,ACTIVE,COMBINED}_EXPANSION_STATS
- bool relativeMetric

  flag indicating the use of relative scaling in refinement metrics
- RealVector dimPrefSpec

  user specification for dimension_preference
- SizetArray collocPtsSeqSpec

user specification of number of initial samples per model instance, including adaptive cases where an optimal sample profile is the target of iteration (e.g., multilevel_regression())

- Real collocRatio

  factor applied to terms^termsOrder in computing number of regression points, either user-specified or inferred

- Real termsOrder

  exponent applied to number of expansion terms for computing number of regression points (usually 1)

- int randomSeed

  seed for random number generator (used for regression with LHS and sub-sampled tensor grids, as well as for expansionSampler)

- SizetArray randomSeedSeqSpec

  user specification for seed_sequence

- bool fixedSeed

  don't continue an existing random number sequence, rather reset seed each time within some sampling-based iteration

- size_t mlmfIter

  top level iteration counter in adaptive NonDExpansion ML/MF algorithms, allowing special updating logic for some sequence handlers

- bool allVars

  flag for combined variable expansions which include a non-probabilistic subset (design, epistemic, state)

- bool tensorRegression

  option for regression FT using a filtered set of tensor-product quadrature points

- short multilevAllocControl

  type of sample allocation scheme for discretization levels / model forms within multilevel / multifidelity methods

- short multilevDiscrepEmulation

  emulation approach for multilevel / multifidelity discrepancy: distinct or recursive

- SizetArray NLev

  number of samples allocated to each level of a discretization/model hierarchy within multilevel/multifidelity methods

- Real equivHFEvals

  equivalent number of high fidelity evaluations accumulated using samples across multiple model forms and/or discretization levels

- Real kappaEstimatorRate

  rate parameter for allocation by ESTIMATOR_VARIANCE in multilevel_regression()

- Real gammaEstimatorScale

  scale parameter for allocation by ESTIMATOR_VARIANCE in multilevel_regression()

- int numSamplesOnModel

  number of truth samples performed on g_u_model to form the expansion

- int numSamplesOnExpansion

  number of approximation samples performed on the polynomial expansion in order to estimate probabilities

- bool nestedRules

  flag for indicating state of `nested` and `non_nested` overrides of default rule nesting, which depends on the type of integration driver; this is defined in construct_{quadrature,sparse_grid}(), such that override attributes (defined in ctors) must be used upstream

- short ruleNestingOverride

  user override of default rule nesting: NO_NESTING_OVERRIDE, NESTED, or NON_NESTED

- short ruleGrowthOverride

  user override of default rule growth: NO_GROWTH_OVERRIDE, RESTRICTED, or UNRESTRICTED

- bool piecewiseBasis

  flag for `piecewise` specification, indicating usage of local basis polynomials within the stochastic expansion

- bool useDerivs

  flag for `use_derivatives` specification, indicating usage of derivative data (with respect to expansion variables) to enhance the calculation of the stochastic expansion.

- RealVector initialPtU

stores the initial variables data in u-space

- short refineType

  refinement type: NO_REFINEMENT, P_REFINEMENT, or H_REFINEMENT

- short refineControl

  refinement control: NO_CONTROL, UNIFORM_CONTROL, LOCAL_ADAPTIVE_CONTROL, DIMENSION_ADAPTIVE_CONTROL_SOBOL, DIMENSION_ADAPTIVE_CONTROL_DECAY, or DIMENSION_ADAPTIVE_CONTROL_GENERALIZED

- short refineMetric

  refinement metric: NO_METRIC, COVARIANCE_METRIC, LEVEL_STATS_METRIC, or MIXED_STATS_METRIC

- short covarianceControl

  enumeration for controlling response covariance calculation and output: {DEFAULT,DIAGONAL,FULL}_COVARIANCE

- unsigned short softConvLimit

  number of consecutive iterations within tolerance required to indicate soft convergence

- RealSymMatrix respCovariance

  symmetric matrix of analytic response covariance (full response covariance option)

- RealVector respVariance

  vector of response variances (diagonal response covariance option)

- RealVector statsStar

  stats of the best refinement candidate for the current model indices

- size_t numUncertainQuant

  number of invocations of core_run()

Private Member Functions

- void initialize_counts ()

  initialize data based on variable counts

- void aggregated_models_mode ()

  set response mode to AGGREGATED_MODELS and recur response size updates

- void bypass_surrogate_mode ()

  set response mode to BYPASS_SURROGATE and recur response size updates

- void multifidelity_reference_expansion ()

  generate a set of reference expansions across a model hierarchy

- void multifidelity_individual_refinement ()

  separately refine each of the multifidelity reference expansions

- void multifidelity_integrated_refinement ()

  refine each of the multifidelity reference expansions within an integrated competition

- void reduce_total_sobol_sets (RealVector &avg_sobol)

  compute average of total Sobol' indices (from VBD) across the response set for use as an anisotropy indicator

- void reduce_decay_rate_sets (RealVector &min_decay)

  compute minimum of spectral coefficient decay rates across the response set for use as an anisotropy indicator

- void print_refinement_diagnostics (std::ostream &s)

  print additional refinement diagnostics not covered by compute_∗_metric()

- size_t increment_sets (Real &delta_star, bool revert, bool print_metric)

  perform an adaptive refinement increment using generalized sparse grids

- void finalize_sets (bool converged_within_tol, bool reverted=false)

  finalization of adaptive refinement using generalized sparse grids

- void select_candidate (size_t best_candidate)

  promote selected candidate into reference grid + expansion

- void select_index_set_candidate (std::set< UShortArray >::const_iterator cit_star)

  promote selected index set candidate into reference grid + expansion

- void select_increment_candidate ()

  promote selected refinement increment candidate into reference grid + expansion
- void compute_analytic_statistics ()

  analytic portion of compute_statistics() from post-processing of expansion coefficients (used for FINAL_RESULTS)
- void compute_numerical_statistics ()

  numerical portion of compute_statistics() from sampling on the expansion (used for FINAL_RESULTS)
- void compute_numerical_stat_refinements (RealVectorArray &imp_sampler_stats, RealRealPairArray &min-_max_fns)

  refinements to numerical probability statistics from importanceSampler
- void define_sampler_asv (ShortArray &sampler_asv)

  helper to define the expansionSampler's data requests when sampling on the expansion
- void run_sampler (const ShortArray &sampler_asv, RealVector &exp_sampler_stats)

  helper to run the expansionSampler and compute its statistics
- void refine_sampler (RealVectorArray &imp_sampler_stats, RealRealPairArray &min_max_fns)

  helper to refine the results from expansionSampler with importance sampling (for probability levels) or bounds post-processing (for PDFs)
- void print_moments (std::ostream &s)

  print expansion and numerical moments
- void print_local_sensitivity (std::ostream &s)

  print local sensitivities evaluated at initialPtU

Private Attributes

- RealMatrix expGradsMeanX

  derivative of the expansion with respect to the x-space variables evaluated at the means (used as uncertainty importance metrics)
- size_t maxRefineIterations

  maximum number of uniform/adaptive refinement iterations (specialization of maxIterations)
- size_t maxSolverIterations

  maximum number of regression solver iterations (specialization of maxIterations)
- bool vbdFlag

  flag indicating the activation of variance-bsaed decomposition for computing Sobol' indices
- unsigned short vbdOrderLimit

  limits the order of interactions within the component Sobol' indices
- Real vbdDropTol

  tolerance for omitting output of small VBD indices

Additional Inherited Members

14.142.1 Detailed Description

Base class for polynomial chaos expansions (PCE), stochastic collocation (SC) and functional tensor train (FT)

The NonDExpansion class provides a base class for methods that use polynomial expansions to approximate the effect of parameter uncertainties on response functions of interest.

14.142.2 Member Function Documentation

14.142.2.1 const Model & algorithm_space_model ( ) const [inline], [virtual]

default definition that gets redefined in selected derived Minimizers

Reimplemented from Analyzer.

References NonDExpansion::uSpaceModel.

Referenced by AdaptedBasisModel::compute_subspace(), and AdaptedBasisModel::get_sub_model().

14.142.2.2 void infer_pilot_sample (size_t *num_steps*, SizetArray & *delta_N_l*) [virtual]

Default implementation redefined by Multilevel derived classes.

Reimplemented in NonDMultilevelPolynomialChaos, and NonDMultilevelFunctionTrain.

References Dakota::abort_handler().

Referenced by NonDExpansion::multilevel_regression().

14.142.2.3 void increment_specification_sequence ( ) [protected], [virtual]

increment the input specification sequence and assign values

Default implementation redefined by Multilevel derived classes.

Reimplemented in NonDMultilevelPolynomialChaos, NonDMultilevelFunctionTrain, and NonDMultilevelStoch-Collocation.

References Dakota::abort_handler().

Referenced by NonDExpansion::multifidelity_reference_expansion().

14.142.2.4 void update_expansion ( ) [protected], [virtual]

update an expansion; avoids overhead in compute_expansion()

leave sampler_set, expansion flags, and distribution parameter settings as set previously by compute_expansion(); there should be no need to update these for an expansion refinement.

References Model::append_approximation(), NonDIntegration::evaluate_grid_increment(), NonDExpansion::expansionCoeffsApproach, NonDExpansion::increment_grid(), Iterator::iterator_rep(), Model::push_approximation(), Model::push_available(), NonDIntegration::push_grid_increment(), Model::rebuild_approximation(), Model::subordinate_iterator(), Model::update_approximation(), and NonDExpansion::uSpaceModel.

Referenced by NonDExpansion::core_refinement(), and NonDExpansion::multilevel_regression().

14.142.2.5 Real compute_covariance_metric (bool *revert*, bool *print_metric*) [protected], [virtual]

compute 2-norm of change in response covariance

computes the default refinement metric based on change in respCovariance

Reimplemented in NonDStochCollocation.

References NonDExpansion::compute_moments(), NonDExpansion::compute_off_diagonal_covariance(), NonDExpansion::covarianceControl, NonDExpansion::print_covariance(), NonDExpansion::relativeMetric, NonDExpansion::respCovariance, and NonDExpansion::respVariance.

Referenced by NonDStochCollocation::compute_covariance_metric(), NonDExpansion::core_refinement(), and NonDExpansion::increment_sets().

14.142.2.6 Real compute_level_mappings_metric (bool *revert,* bool *print_metric*) [protected], [virtual]

compute 2-norm of change in final statistics

computes a "goal-oriented" refinement metric employing computed*Levels

Reimplemented in NonDStochCollocation.

References NonDExpansion::compute_level_mappings(), NonD::print_level_mappings(), NonD::pull_level_mappings(), NonD::push_level_mappings(), NonDExpansion::relativeMetric, and NonD::totalLevelRequests.

Referenced by NonDStochCollocation::compute_level_mappings_metric(), NonDExpansion::core_refinement(), and NonDExpansion::increment_sets().

14.142.2.7 void compute_statistics (short *results_state* = FINAL_RESULTS) [protected], [virtual]

calculate analytic and numerical statistics from the expansion, supporting {REFINEMENT,INTERMEDIATE,FINAL}_RESULTS modes

Calculate analytic and numerical statistics from the expansion and log results within final_stats for use in OUU.

References ResultsManager::active(), NonDExpansion::allVars, NonDExpansion::archive_coefficients(), NonDExpansion::archive_moments(), NonDExpansion::archive_sobol_indices(), NonDExpansion::compute_analytic_statistics(), NonDExpansion::compute_level_mappings(), NonDExpansion::compute_moments(), NonDExpansion::compute_numerical_statistics(), NonDExpansion::compute_off_diagonal_covariance(), Model::continuous_variable_labels(), Model::continuous_variables(), NonDExpansion::covarianceControl, NonDExpansion::initialPtU, ResultsManager::insert(), Iterator::iteratedModel, NonDExpansion::refineMetric, Model::response_labels(), Iterator::resultsDB, Iterator::resultsNames, Iterator::run_identifier(), NonD::totalLevelRequests, NonDExpansion::update_final_statistics(), NonDExpansion::uSpaceModel, and NonDExpansion::vbdFlag.

Referenced by NonDExpansion::core_refinement(), NonDMultilevelStochCollocation::core_run(), NonDExpansion::core_run(), NonDMultilevelFunctionTrain::core_run(), NonDMultilevelPolynomialChaos::core_run(), NonDExpansion::increment_sets(), NonDExpansion::multifidelity_individual_refinement(), and NonDExpansion::multifidelity_reference_expansion().

14.142.2.8 void update_samples_from_order_decrement ( ) [protected], [virtual]

update (restore previous) numSamplesOnModel after an order decrement

Default implementation: increment/decrement update process is identical

References NonDExpansion::update_samples_from_order_increment().

Referenced by NonDExpansion::decrement_order_and_grid().

14.142.2.9 int seed_sequence (size_t *index*) const [inline], [protected]

return random seed for index within model sequence

extract an active seed from a seed sequence

References NonDExpansion::fixedSeed, NonDExpansion::mlmfIter, and NonDExpansion::randomSeedSeqSpec.

Referenced by NonDMultilevelStochCollocation::first_seed(), NonDMultilevelFunctionTrain::first_seed(), NonDMultilevelPolynomialChaos::first_seed(), NonDMultilevelStochCollocation::random_seed(), NonDMultilevelFunctionTrain::random_seed(), NonDMultilevelPolynomialChaos::random_seed(), and NonDExpansion::update_u_space_sampler().

14.142.2.10 void increment_order_and_grid ( ) [protected]

uniformly increment the expansion order and structured/unstructured grid (PCE and FT)

Used for uniform refinement of regression-based PCE / FT.

References SharedApproxData::increment_order(), Iterator::iterator_rep(), NonDExpansion::numSamplesOnModel, NonDQuadrature::samples(), Model::shared_approximation(), Model::subordinate_iterator(), NonDExpansion::tensorRegression, NonDExpansion::update_model_from_samples(), NonDExpansion::update_samples_from_order_increment(), and NonDExpansion::uSpaceModel.

Referenced by NonDExpansion::increment_grid().

14.142.2.11 void decrement_order_and_grid ( ) [protected]

uniformly decrement the expansion order and structured/unstructured grid (PCE and FT)

Used for uniform de-refinement of regression-based PCE / FT.

References SharedApproxData::decrement_order(), Iterator::iterator_rep(), NonDExpansion::numSamplesOnModel, NonDQuadrature::samples(), Model::shared_approximation(), Model::subordinate_iterator(), NonDExpansion::tensorRegression, NonDExpansion::update_model_from_samples(), NonDExpansion::update_samples_from_order_decrement(), and NonDExpansion::uSpaceModel.

Referenced by NonDExpansion::decrement_grid().

14.142.3 Member Data Documentation

14.142.3.1 bool useDerivs [protected]

flag for `use_derivatives` specification, indicating usage of derivative data (with respect to expansion variables) to enhance the calculation of the stochastic expansion.

This is part of the method specification since the instantiation of the global data fit surrogate is implicit with no user specification. This behavior is distinct from the usage of response derivatives with respect to auxilliary variables (design, epistemic) for computing derivatives of aleatory expansion statistics with respect to these variables.

Referenced by NonDExpansion::compute_expansion(), NonDExpansion::configure_pecos_options(), NonDPolynomialChaos::ratio_samples_to_order(), NonDStochCollocation::resolve_inputs(), NonDPolynomialChaos::resolve_inputs(), NonDExpansion::terms_ratio_to_samples(), and NonDExpansion::terms_samples_to_ratio().

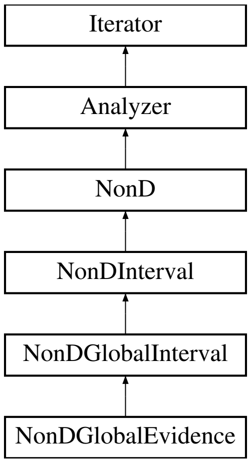
The documentation for this class was generated from the following files:

- NonDExpansion.hpp
- NonDExpansion.cpp

14.143 NonDGlobalEvidence Class Reference

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

Inheritance diagram for NonDGlobalEvidence:



Public Member Functions

- NonDGlobalEvidence (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDGlobalEvidence ()

  destructor
- void initialize ()

  perform any required initialization
- void set_cell_bounds ()

  set the optimization variable bounds for each cell
- void get_best_sample (bool maximize, bool eval_approx)

  determine truthFnStar and approxFnStar
- void post_process_cell_results (bool maximize)

  post-process a cell minimization/maximization result
- void post_process_response_fn_results ()

  post-process the interval computed for a response function
- void post_process_final_results ()

  perform final post-processing

Additional Inherited Members

14.143.1 Detailed Description

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

The NonDEvidence class implements the propagation of epistemic uncertainty using Dempster-Shafer theory of evidence. In this approach, one assigns a set of basic probability assignments (BPA) to intervals defined for the uncertain variables. Input interval combinations are calculated, along with their BPA. Currently, the response function is evaluated at a set of sample points, then a response surface is constructed which is sampled extensively to find the minimum and maximum within each input interval cell, corresponding to the belief and plausibility within that cell, respectively. This data is then aggregated to calculate cumulative distribution functions for belief and plausibility.

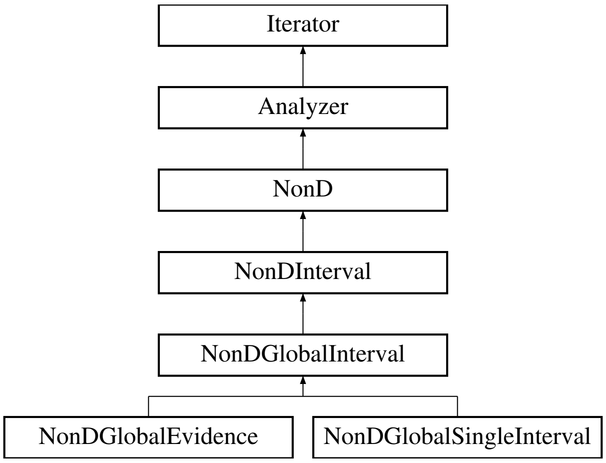
The documentation for this class was generated from the following files:

- NonDGlobalEvidence.hpp
- NonDGlobalEvidence.cpp

14.144 NonDGlobalInterval Class Reference

Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

Inheritance diagram for NonDGlobalInterval:



Public Member Functions

- NonDGlobalInterval (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDGlobalInterval ()

  destructor
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- void core_run ()

  Performs an optimization to determine interval bounds for an entire function or interval bounds on a particular statistical estimator.
- const Model & algorithm_space_model () const

Protected Member Functions

- virtual void initialize ()

  perform any required initialization
- virtual void set_cell_bounds ()

  set the optimization variable bounds for each cell
- virtual void get_best_sample (bool maximize, bool eval_approx)

  determine truthFnStar and approxFnStar
- virtual void post_process_cell_results (bool maximize)

  post-process a cell minimization/maximization result
- virtual void post_process_response_fn_results ()

  post-process the interval computed for a response function
- virtual void post_process_final_results ()

perform final post-processing

- void post_process_run_results (bool maximize)

  post-process an optimization execution: output results, update convergence controls, and update GP approximation
- void evaluate_response_star_truth ()

  evaluate the truth response at the optimal variables solution and update the GP with the new data

Protected Attributes

- Iterator daceIterator

  LHS iterator for constructing initial GP for all response functions.
- Model fHatModel

  GP model of response, one approximation per response function.
- Iterator intervalOptimizer

  optimizer for solving surrogate-based subproblem: NCSU DIRECT optimizer for maximizing expected improvement or mixed EA if discrete variables.
- Model intervalOptModel

  recast model which formulates the surrogate-based optimization subproblem (recasts as design problem; may assimilate mean and variance to enable max(expected improvement))
- Real approxFnStar

  approximate response corresponding to minimum/maximum truth response
- Real truthFnStar

  minimum/maximum truth response function value

Static Private Member Functions

- static void EIF_objective_min (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the objective function in the Expected Improvement Function (EIF) for minimizing the GP
- static void EIF_objective_max (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the objective function in the Expected Improvement Function (EIF) for maximizing the GP
- static void extract_objective (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used to extract the active objective function when optimizing for an interval lower or upper bound (non-EIF formulations). The sense of the optimization is set separately.

Private Attributes

- const int seedSpec

  the user seed specification (default is 0)
- int numSamples

  the number of samples used in the surrogate
- String rngName

  name of the random number generator
- bool gpModelFlag

  flag indicating use of GP surrogate emulation
- bool eifFlag

  flag indicating use of maximized expected improvement for GP iterate selection
- unsigned short improvementConvergeCntr

  counter for number of successive iterations that the iteration improvement is less than the convergenceTol
- unsigned short improvementConvergeLimit

counter for number of successive iterations that the iteration improvement is less than the convergenceTol

- Real distanceTol

  tolerance for L_2 change in optimal solution

- unsigned short distanceConvergeCntr

  counter for number of successive iterations that the L_2 change in optimal solution is less than the convergenceTol

- unsigned short distanceConvergeLimit

  counter for number of successive iterations that the L_2 change in optimal solution is less than the convergenceTol

- RealVector prevCVStar

  stores previous optimal point for continuous variables; used for assessing convergence

- IntVector prevDIVStar

  stores previous optimal point for discrete integer variables; used for assessing convergence

- RealVector prevDRVStar

  stores previous optimal point for discrete real variables; used for assessing convergence

- Real prevFnStar

  stores previous solution value for assessing convergence

- size_t globalIterCntr

  global iteration counter for number of surrogate-based min/max solves

- bool boundConverged

  flag indicating convergence of a minimization or maximization cycle

- bool allResponsesPerIter

  flag for maximal response extraction (all response values obtained on each function call)

- short dataOrder

  order of the data used for surrogate construction, in ActiveSet request vector 3-bit format; user may override responses spec

Static Private Attributes

- static NonDGlobalInterval * nondGIInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

14.144.1 Detailed Description

Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

The NonDGlobalInterval class supports global nongradient-based optimization apporaches to determining interval bounds for epistemic UQ. The interval bounds may be on the entire function in the case of pure interval analysis (e.g. intervals on input = intervals on output), or the intervals may be on statistics of an "inner loop" aleatory analysis such as intervals on means, variances, or percentile levels. The preliminary implementation will use a Gaussian process surrogate to determine interval bounds.

14.144.2 Member Function Documentation

14.144.2.1 const Model & algorithm_space_model ( ) const [inline], [virtual]

default definition that gets redefined in selected derived Minimizers

Reimplemented from Analyzer.

References NonDGlobalInterval::fHatModel.

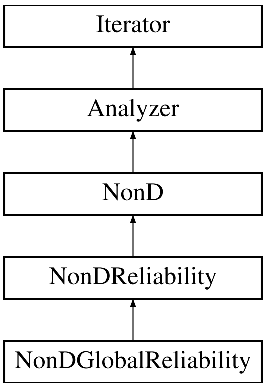
The documentation for this class was generated from the following files:

- NonDGlobalInterval.hpp
- NonDGlobalInterval.cpp

14.145 NonDGlobalReliability Class Reference

Class for global reliability methods within DAKOTA/UQ.

Inheritance diagram for NonDGlobalReliability:



Public Member Functions

- NonDGlobalReliability (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDGlobalReliability ()

  destructor
- bool resize ()

  reinitializes iterator based on new variable size
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()

  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final iterator results

Private Member Functions

- void optimize_gaussian_process ()

  construct the GP using EGO/SKO
- void importance_sampling ()

  perform multimodal adaptive importance sampling on the GP
- void get_best_sample ()

determine current best solution from among sample data for expected imporovement function in Performance Measure Approach (PMA)

- Real constraint_penalty (const Real &constraint, const RealVector &c_variables)

  calculate the penalty to be applied to the PMA constraint value
- Real expected_improvement (const RealVector &expected_values, const Variables &recast_vars)

  expected improvement function for the GP
- Real expected_feasibility (const RealVector &expected_values, const Variables &recast_vars)

  expected feasibility function for the GP
- void x_truth_evaluation (short mode)

  evaluate iteratedModel at current point to collect x-space truth data
- void x_truth_evaluation (const RealVector &c_vars_u, short mode)

  evaluate iteratedModel at specified point to collect x-space truth data
- void u_truth_evaluation (const RealVector &c_vars_u, short mode)

  evaluate uSpaceModel in BYPASS_SURROGATE mode to collect u-space truth data at specified point
- void u_evaluation (const RealVector &c_vars_u, short mode)

  evaluate uSpaceModel to collect u-space surrogate data at specified point

Static Private Member Functions

- static void EIF_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the objective function in the Expected Improvement (EIF) problem formulation for PMA
- static void EFF_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the objective function in the Expected Feasibility (EFF) problem formulation for RIA

Private Attributes

- Real fnStar

  minimum penalized response from among true function evaluations
- short meritFunctionType

  type of merit function used to penalize sample data
- Real lagrangeMult

  Lagrange multiplier for standard Lagrangian merit function.
- Real augLagrangeMult

  Lagrange multiplier for augmented Lagrangian merit function.
- Real penaltyParameter

  penalty parameter for augmented Lagrangian merit funciton
- Real lastConstraintViolation

  constraint violation at last iteration, used to determine if the current iterate should be accepted (must reduce violation)
- bool lastIterateAccepted

  flag to determine if last iterate was accepted this controls update of parameters for augmented Lagrangian merit fn
- short dataOrder

  order of the data used for surrogate construction, in ActiveSet request vector 3-bit format; user may override responses spec

Static Private Attributes

- static NonDGlobalReliability ∗ nondGlobRelInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

14.145.1 Detailed Description

Class for global reliability methods within DAKOTA/UQ.

The NonDGlobalReliability class implements EGO/SKO for global MPP search, which maximizes an expected improvement function derived from Gaussian process models. Once the limit state has been characterized, a multimodal importance sampling approach is used to compute probabilities.

14.145.2 Member Function Documentation

14.145.2.1 void pre_run ( ) [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

References Model::initialize_mapping(), Iterator::methodPCIter, NonD::miPLIndex, NonDReliability::mppModel, Analyzer::pre_run(), and Model::update_from_subordinate_model().

14.145.2.2 void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References NonDGlobalReliability::importance_sampling(), NonDGlobalReliability::nondGlobRelInstance, and NonDGlobalReliability::optimize_gaussian_process().

14.145.2.3 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

References NonD::cdfFlag, NonD::computedGenRelLevels, NonD::computedProbLevels, NonD::computedRespLevels, Iterator::iteratedModel, Analyzer::numFunctions, NonD::print_densities(), Model::response_labels(), and Dakota::write_precision.

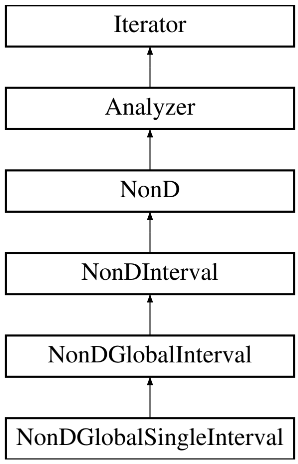
The documentation for this class was generated from the following files:

- NonDGlobalReliability.hpp
- NonDGlobalReliability.cpp

14.146 NonDGlobalSingleInterval Class Reference

Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

Inheritance diagram for NonDGlobalSingleInterval:



Public Member Functions

- NonDGlobalSingleInterval (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDGlobalSingleInterval ()

  destructor

Protected Member Functions

- void initialize ()

  perform any required initialization
- void post_process_cell_results (bool maximize)

  post-process a cell minimization/maximization result
- void get_best_sample (bool maximize, bool eval_approx)

  determine truthFnStar and approxFnStar

Private Attributes

- size_t statCntr

  counter for finalStatistics

Additional Inherited Members

14.146.1 Detailed Description

Class for using global nongradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

The NonDGlobalSingleInterval class supports global nongradient-based optimization apporaches to determining interval bounds for epistemic UQ. The interval bounds may be on the entire function in the case of pure interval analysis (e.g. intervals on input = intervals on output), or the intervals may be on statistics of an "inner loop" aleatory analysis such as intervals on means, variances, or percentile levels. The preliminary implementation will use a Gaussian process surrogate to determine interval bounds.

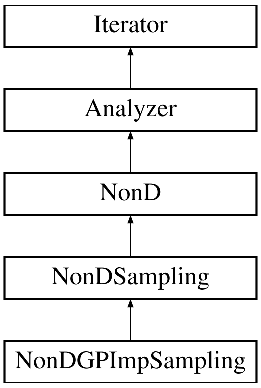
The documentation for this class was generated from the following files:

- NonDGlobalSingleInterval.hpp
- NonDGlobalSingleInterval.cpp

14.147 NonDGPImpSampling Class Reference

Class for the Gaussian Process-based Importance Sampling method.

Inheritance diagram for NonDGPImpSampling:



Public Member Functions

- NonDGPImpSampling (ProblemDescDB &problem_db, Model &model)

  standard constructor
- ∼NonDGPImpSampling ()

  destructor
- bool resize ()

  reinitializes iterator based on new variable size
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- void core_run ()

  perform the GP importance sampling and return probability of failure
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final statistics
- Real final_probability ()

  returns the probability calculated by the importance sampling

Private Member Functions

- RealVector calcExpIndicator (const int respFnCount, const Real respThresh)

  function to calculate the expected indicator probabilities
- Real calcExpIndPoint (const int respFnCount, const Real respThresh, const RealVector this_mean, const RealVector this_var)

  function to calculate the expected indicator probabilities for one point
- void calcRhoDraw ()

function to update the rhoDraw data, adding x values and rho draw values

- RealVector drawNewX (int this_k)

  function to pick the next X value to be evaluated by the Iterated model

Private Attributes

- Iterator gpBuild

  LHS iterator for building the initial GP.

- Iterator gpEval

  LHS iterator for sampling on the GP.

- Model gpModel

  GP model of response, one approximation per response function.

- Iterator sampleRhoOne

  LHS iterator for sampling from the rhoOneDistribution.

- int numPtsAdd

  the number of points added to the original set of LHS samples

- int numPtsTotal

  the total number of points

- int numEmulEval

  the number of points evaluated by the GP each iteration

- Real finalProb

  the final calculated probability (p)

- RealVectorArray gpCvars

  Vector to hold the current values of the current sample inputs on the GP.

- RealVectorArray gpMeans

  Vector to hold the current values of the current mean estimates for the sample values on the GP.

- RealVectorArray gpVar

  Vector to hold the current values of the current variance estimates for the sample values on the GP.

- RealVector expIndicator

  Vector to hold the expected indicator values for the current GP samples.

- RealVector rhoDraw

  Vector to hold the rhoDraw values for the current GP samples.

- RealVector normConst

  Vector to hold the normalization constant calculated for each point added.

- RealVector indicator

  IntVector to hold indicator for actual simulation values vs. threshold.

- RealVectorArray xDrawThis

  xDrawThis, appended to locally to hold the X values of emulator points chosen

- RealVector expIndThis

  expIndThis, appended locally to hold the expected indicator

- RealVector rhoDrawThis

  rhoDrawThis, appended locally to hold the rhoDraw density for calculating draws

- RealVector rhoMix

  rhoMix, mixture density

- RealVector rhoOne

  rhoOne, original importance density

Additional Inherited Members

14.147.1 Detailed Description

Class for the Gaussian Process-based Importance Sampling method.

The NonDGPImpSampling implements a method developed by Keith Dalbey that uses a Gaussian process surrogate in the calculation of the importance density. Specifically, the mean and variance of the GP prediction are used to calculate an expected value that a particular point fails, and that is used as part of the computation of the "draw distribution." The normalization constants and the mixture distribution used are defined in (need to get SAND report).

14.147.2 Constructor & Destructor Documentation

14.147.2.1 NonDGPImpSampling (ProblemDescDB & *problem_db*, Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Response::active_set(), Iterator::assign_rep(), Model::assign_rep(), NonD::construct_lhs(), Model::current_response(), ProblemDescDB::get_bool(), ProblemDescDB::get_int(), ProblemDescDB::get_string(), ProblemDescDB::get_ushort(), NonDGPImpSampling::gpBuild, NonDGPImpSampling::gpEval, NonDGPImpSampling::gpModel, Model::gradient_type(), Model::hessian_type(), NonD::initialize_final_statistics(), Iterator::iteratedModel, Iterator::maxIterations, NonDGPImpSampling::numEmulEval, NonDGPImpSampling::numPtsAdd, NonDSampling::numSamples, Iterator::outputLevel, Iterator::probDescDB, NonDSampling::randomSeed, ActiveSet::request_values(), NonDSampling::rngName, NonDGPImpSampling::sampleRhoOne, NonDSampling::sampleType, NonDSampling::samplingVarsMode, NonDSampling::statsFlag, Dakota::SZ_MAX, NonDSampling::vary_pattern(), and NonDSampling::varyPattern.

14.147.3 Member Function Documentation

14.147.3.1 void core_run ( ) [virtual]

perform the GP importance sampling and return probability of failure

Calculate the failure probabilities for specified probability levels using Gaussian process based importance sampling.

Reimplemented from Iterator.

References Model::acv(), Iterator::all_responses(), Analyzer::all_samples(), Iterator::all_samples(), Model::append_approximation(), Model::approximation_data(), Model::approximation_variances(), Model::build_approximation(), NonDGPImpSampling::calcExpIndicator(), NonDGPImpSampling::calcExpIndPoint(), NonDGPImpSampling::calcRhoDraw(), NonD::cdfFlag, NonD::computedProbLevels, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Model::current_response(), Model::current_variables(), NonDGPImpSampling::drawNewX(), Model::evaluate(), Model::evaluation_id(), NonDGPImpSampling::expIndicator, NonDGPImpSampling::expIndThis, NonDGPImpSampling::finalProb, Response::function_values(), NonDGPImpSampling::gpCvars, NonDGPImpSampling::gpEval, NonDGPImpSampling::gpMeans, NonDGPImpSampling::gpModel, NonDGPImpSampling::gpVar, NonDGPImpSampling::indicator, NonD::initialize_level_mappings(), Iterator::iteratedModel, Iterator::methodPCIter, NonD::miPLIndex, NonDGPImpSampling::normConst, NonDGPImpSampling::numEmulEval, Analyzer::numFunctions, NonDGPImpSampling::numPtsAdd, NonDGPImpSampling::numPtsTotal, NonDSampling::numSamples, Iterator::outputLevel, Model::pop_approximation(), NonD::requestedRespLevels, NonDGPImpSampling::rhoDraw, NonDGPImpSampling::rhoDrawThis, NonDGPImpSampling::rhoMix, NonDGPImpSampling::rhoOne, Iterator::run(), NonDGPImpSampling::sampleRhoOne, and NonDGPImpSampling::xDrawThis.

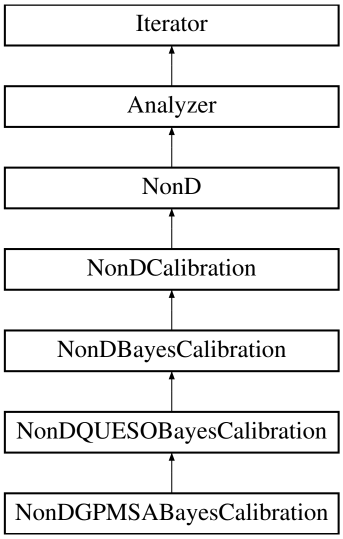
The documentation for this class was generated from the following files:

- NonDGPImpSampling.hpp
- NonDGPImpSampling.cpp

14.148 NonDGPMSABayesCalibration Class Reference

Generates posterior distribution on model parameters given experiment data.

Inheritance diagram for NonDGPMSABayesCalibration:



Public Member Functions

- NonDGPMSABayesCalibration (ProblemDescDB &problem_db, Model &model)

    constructor
- ∼NonDGPMSABayesCalibration ()

    destructor

Protected Member Functions

- void derived_init_communicators (ParLevLIter pl_iter)

    derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

    derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

    derived class contributions to freeing the communicators associated with this Iterator instance
- void calibrate ()

    performs a forward uncertainty propagation by using GPM/SA to generate a posterior distribution on parameters given a set of simulation parameter/response data, a set of experimental data, and additional variables to be specified here.
- void init_queso_solver ()

    specialization to initialize the inverse problem and posterior
- void acquire_simulation_data (RealMatrix &sim_data)

    Populate simulation data (run design of experiments or load build data)
- void overlay_proposal_covariance (QUESO::GslMatrix &full_prop_cov) const

    fill the full proposal covariance, inlcuding hyperparameter entries with user-specified or default theta covariance information

- void fill_simulation_data ()

  populate the simulation data, calculating and applying scaling if needed
- void fill_experiment_data ()

  populate the experiment data, applying scaling if needed
- void overlay_initial_params (QUESO::GslVector &full_param_initials)

  overlay the Dakota user's initial parameters on the full GPMSA vector of parameters
- void cache_acceptance_chain ()

  retrieve the chain from QUESO and populate acceptanceChain / acceptedFnVals
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final iterator results

Protected Attributes

- int buildSamples

  number of samples of the simulation to construct the GP
- String approxImportFile

  name of file from which to import build points to build GP
- unsigned short approxImportFormat

  build data import tabular format
- bool approxImportActiveOnly

  import active variables only
- unsigned int userConfigVars

  number of user-specified configuration (scenario) vars
- unsigned int gpmsaConfigVars

  number of config vars presented to GPMSA (minimum 1)
- bool gpmsaNormalize

  whether to apply GPMSA-internal variable and data normalization
- std::shared_ptr
  < QUESO::VectorSpace
  < QUESO::GslVector,
  QUESO::GslMatrix > > configSpace

  vector space defining the scenario (configuration) variables
- std::shared_ptr
  < QUESO::VectorSpace
  < QUESO::GslVector,
  QUESO::GslMatrix > > nEtaSpace

  vector space defining the output (response) space for the simulations
- std::shared_ptr
  < QUESO::VectorSpace
  < QUESO::GslVector,
  QUESO::GslMatrix > > experimentSpace

  vector space defining the output (response) space for the experiments
- std::shared_ptr
  < QUESO::GPMSAOptions > gpmsaOptions

  Configuration options for the GPMSA solver.
- std::shared_ptr
  < QUESO::GPMSAFactory
  < QUESO::GslVector,
  QUESO::GslMatrix > > gpmsaFactory

  core factory that manages a GP-based likelihood

Private Attributes

- Iterator lhsIter

  LHS iterator for generating samples for GP.

Static Private Attributes

- static NonDGPMSABayesCalibration ∗ nonDGPMSAInstance

  Pointer to current class instance for use in static callback functions.

Additional Inherited Members

14.148.1 Detailed Description

Generates posterior distribution on model parameters given experiment data.

This class provides a wrapper for the functionality provided in the Los Alamos National Laboratory code called GPM/SA (Gaussian Process Models for Simulation Analysis). Although this is a code that provides input/output mapping, it DOES NOT provide the mapping that we usually think of in the NonDeterministic class hierarchy in DAKOTA, where uncertainty in parameter inputs are mapped to uncertainty in simulation responses. Instead, this class takes a pre-existing set of simulation data as well as experimental data, and maps priors on input parameters to posterior distributions on those input parameters, according to a likelihood function. The goal of the MCMC sampling is to produce posterior values of parameter estimates which will produce simulation response values that "match well" to the experimental data. The MCMC is an integral part of the calibration. The data structures in GPM/SA are fairly detailed and nested. Part of this prototyping exercise is to determine what data structures need to be specified and initialized in DAKOTA and sent to GPM/SA, and what data structures will be returned.

14.148.2 Constructor & Destructor Documentation

14.148.2.1 NonDGPMSABayesCalibration (ProblemDescDB & *problem_db,* Model & *model*)

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDGPMSABayesCalibration::approxImportActiveOnly, NonDGPMSA-BayesCalibration::approxImportFile, Iterator::assign_rep(), NonDGPMSABayesCalibration::buildSamples, Model-::current_response(), NonDBayesCalibration::emulatorType, NonDCalibration::expData, ProblemDescDB::get-_string(), NonDGPMSABayesCalibration::lhsIter, NonDBayesCalibration::mcmcModel, ExperimentData::num_-experiments(), SharedResponseData::num_field_response_groups(), Iterator::outputLevel, Iterator::probDescDB, NonDBayesCalibration::randomSeed, Response::shared_data(), and NonDGPMSABayesCalibration::userConfig-Vars.

14.148.3 Member Function Documentation

14.148.3.1 void calibrate ( ) [protected], [virtual]

performs a forward uncertainty propagation by using GPM/SA to generate a posterior distribution on parameters given a set of simulation parameter/response data, a set of experimental data, and additional variables to be specified here.

Perform the uncertainty quantification

Implements NonDBayesCalibration.

References NonDQUESOBayesCalibration::advancedOptionsFile, ExperimentData::all_data(), NonDGPMSABayesCalibration::buildSamples, NonDGPMSABayesCalibration::cache_acceptance_chain(), NonDQUESOBayesCalibration::callpMhOptionsValues, NonDGPMSABayesCalibration::configSpace, NonDCalibration::expData, NonDGPMSABayesCalibration::experimentSpace, NonDGPMSABayesCalibration::fill_experiment_data(), NonDGPMSABayesCalibration::fill_simulation_data(), NonDGPMSABayesCalibration::gpmsaConfigVars, NonDGPMSABayesCalibration::gpmsaFactory, NonDGPMSABayesCalibration::gpmsaNormalize, NonDGPMSABayesCalibration::gpmsaOptions, NonDGPMSABayesCalibration::init_queso_solver(), NonDQUESOBayesCalibration::inverseProb, NonDQUESOBayesCalibration::mcmcType, NonDGPMSABayesCalibration::nEtaSpace, NonDGPMSABayesCalibration::nonDGPMSAInstance, NonDQUESOBayesCalibration::nonDQUESOInstance, ExperimentData::num_experiments(), Analyzer::numContinuousVars, Analyzer::numFunctions, NonDBayesCalibration::numHyperparams, Iterator::outputLevel, NonDGPMSABayesCalibration::overlay_initial_params(), NonDGPMSABayesCalibration::overlay_proposal_covariance(), NonDQUESOBayesCalibration::paramSpace, NonDQUESOBayesCalibration::priorRv, NonDQUESOBayesCalibration::quesoEnv, and NonDBayesCalibration::standardizedSpace.

14.148.3.2 void fill_simulation_data ( ) [protected]

populate the simulation data, calculating and applying scaling if needed

simulation data, one row per simulation build sample, columns for calibration variables, configuration variables, function values (duplicates storage, but unifies import vs. DOE cases)

References NonDGPMSABayesCalibration::acquire_simulation_data(), NonDGPMSABayesCalibration::buildSamples, NonDGPMSABayesCalibration::configSpace, NonDGPMSABayesCalibration::gpmsaConfigVars, NonDGPMSABayesCalibration::gpmsaFactory, NonDGPMSABayesCalibration::nEtaSpace, Analyzer::numContinuousVars, Analyzer::numFunctions, NonDQUESOBayesCalibration::paramSpace, and NonDGPMSABayesCalibration::userConfigVars.

Referenced by NonDGPMSABayesCalibration::calibrate().

14.148.3.3 void cache_acceptance_chain ( ) [protected]

retrieve the chain from QUESO and populate acceptanceChain / acceptedFnVals

This is a subset of the base class retrieval, but we can't do the fn value lookups. Eventually should be able to retrieve them from GPMSA.

References NonDBayesCalibration::acceptanceChain, NonDBayesCalibration::acceptedFnVals, NonDBayesCalibration::chainSamples, NonDQUESOBayesCalibration::copy_gsl_partial(), NonDQUESOBayesCalibration::inverseProb, NonDBayesCalibration::mcmcModel, Analyzer::numContinuousVars, Analyzer::numFunctions, NonDBayesCalibration::numHyperparams, Iterator::outputLevel, NonDQUESOBayesCalibration::postRv, Model::probability_transformation(), and NonDBayesCalibration::standardizedSpace.

Referenced by NonDGPMSABayesCalibration::calibrate().

14.148.3.4 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from NonDBayesCalibration.

References NonDBayesCalibration::print_results().

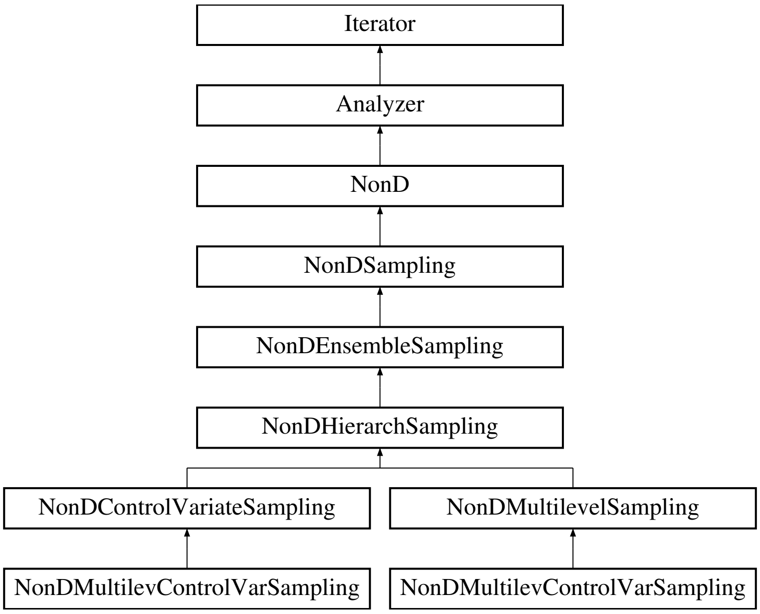
The documentation for this class was generated from the following files:

- NonDGPMSABayesCalibration.hpp
- NonDGPMSABayesCalibration.cpp

14.149 NonDHierarchSampling Class Reference

Performs Hierarch Monte Carlo sampling for uncertainty quantification.

Inheritance diagram for NonDHierarchSampling:



Public Member Functions

- NonDHierarchSampling (ProblemDescDB &problem_db, Model &model)

    standard constructor
- virtual ∼NonDHierarchSampling ()

    destructor (virtual declaration should be redundant with ∼Iterator, but this is top of MLMF diamond so doesn't hurt to be explicit)

Protected Member Functions

- void uncorrected_surrogate_mode ()

    synchronize iteratedModel and activeSet on UNCORRECTED_SURROGATE mode
- void average_online_cost (const RealVector &accum_cost, const SizetArray &num_cost, RealVector &seq_-cost)

    average costs once accumulations are complete
- void accumulate_paired_online_cost (RealVector &accum_cost, SizetArray &num_cost, size_t step)

    recover partial estimates of simulation cost using aggregated (paired) response metadata
- void recover_paired_online_cost (RealVector &seq_cost, size_t step)

    accumulate cost and counts and then perform averaging

Additional Inherited Members

14.149.1 Detailed Description

Performs Hierarch Monte Carlo sampling for uncertainty quantification.

Hierarch Monte Carlo (MLMC) is a variance-reduction technique that utilitizes lower fidelity simulations that have response QoI that are correlated with the high-fidelity response QoI.

14.149.2 Constructor & Destructor Documentation

14.149.2.1 NonDHierarchSampling (ProblemDescDB & *problem_db*, Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDEnsembleSampling::aggregated_models_mode(), NonDEnsembleSampling::costMetadataIndices, ProblemDescDB::get_sza(), Iterator::iteratedModel, Iterator::maxEvalConcurrency, Iterator::method_enum_to_string(), Iterator::methodName, NonDEnsembleSampling::NLev, NonDEnsembleSampling::pilotSamples, Model::subordinate_models(), Model::surrogate_type(), and Dakota::SZ_MAX.

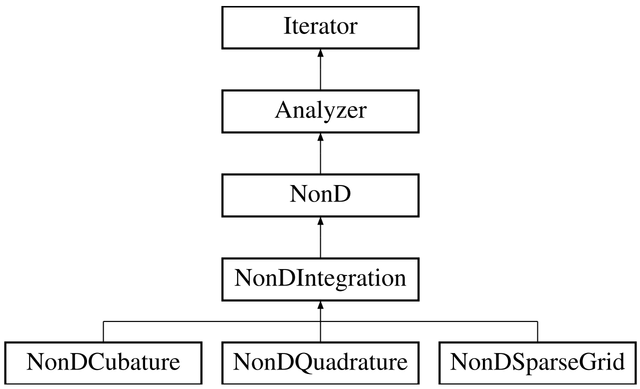
The documentation for this class was generated from the following files:

- NonDHierarchSampling.hpp
- NonDHierarchSampling.cpp

14.150 NonDIntegration Class Reference

Derived nondeterministic class that generates N-dimensional numerical integration points for evaluation of expectation integrals.

Inheritance diagram for NonDIntegration:



Public Member Functions

- virtual void initialize_grid (const std::vector< Pecos::BasisPolynomial > &poly_basis)=0

    initialize integration grid by drawing from polynomial basis settings
- virtual void increment_grid ()=0

    increment SSG level/TPQ order
- virtual void increment_grid_preference (const RealVector &dim_pref)

    increment SSG level/TPQ order and update anisotropy
- virtual void increment_grid_preference ()

    increment SSG level/TPQ order and preserve anisotropy
- virtual void increment_grid_weights (const RealVector &aniso_wts)

    increment SSG level/TPQ order and update anisotropy
- virtual void increment_grid_weights ()

    increment SSG level/TPQ order and preserve anisotropy
- virtual void decrement_grid ()=0

    decrement SSG level/TPQ order

- virtual void evaluate_grid_increment ()

  computes a grid increment and evaluates the new parameter sets
- virtual void push_grid_increment ()

  restores a previously computed grid increment (no new evaluations)
- virtual void pop_grid_increment ()

  removes a previously computed grid increment
- virtual void merge_grid_increment ()

  merges a grid increment into the reference grid
- virtual void update_reference ()

  update reference grid within adaptive grid refinement procedures
- const std::vector
  < Pecos::BasisPolynomial > & polynomial_basis () const

  return IntegrationDriver::polynomialBasis
- std::vector
  < Pecos::BasisPolynomial > & polynomial_basis ()

  return IntegrationDriver::polynomialBasis
- const Pecos::IntegrationDriver & driver () const

  return numIntDriver
- bool resize ()

  reinitializes iterator based on new variable size

Protected Member Functions

- NonDIntegration (ProblemDescDB &problem_db, Model &model)

  constructor
- NonDIntegration (unsigned short method_name, Model &model)

  alternate constructor for instantiations "on the fly"
- NonDIntegration (unsigned short method_name, Model &model, const RealVector &dim_pref)

  alternate constructor for instantiations "on the fly"
- ∼NonDIntegration ()

  destructor
- void core_run ()

  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void print_points_weights (const String &tabular_name)

  output integration points and weights to a tabular file

Protected Attributes

- Pecos::IntegrationDriver numIntDriver

  Pecos utlity class for managing interface to tensor-product grids and VPISparseGrid utilities for Smolyak sparse grids and cubature.
- size_t numIntegrations

  counter for number of integration executions for this object
- RealVector dimPrefSpec

  the user specification for anisotropic dimension preference

Additional Inherited Members

14.150.1 Detailed Description

Derived nondeterministic class that generates N-dimensional numerical integration points for evaluation of expectation integrals.

This class provides a base class for shared code among NonDQuadrature and NonDSparseGrid.

14.150.2 Constructor & Destructor Documentation

14.150.2.1 NonDIntegration (ProblemDescDB & *problem_db,* Model & *model*) [protected]

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification. It is not currently used, as there are not yet separate nond_quadrature/nond_sparse_grid method specifications.

References NonD::initialize_final_statistics().

14.150.2.2 NonDIntegration (unsigned short *method_name,* Model & *model*) [protected]

alternate constructor for instantiations "on the fly"

This alternate constructor is used for on-the-fly generation and evaluation of numerical integration points.

14.150.2.3 NonDIntegration (unsigned short *method_name,* Model & *model,* const RealVector & *dim_pref*) [protected]

alternate constructor for instantiations "on the fly"

This alternate constructor is used for on-the-fly generation and evaluation of numerical integration points.

14.150.3 Member Function Documentation

14.150.3.1 void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Analyzer::evaluate_parameter_sets(), Analyzer::get_parameter_sets(), Iterator::iteratedModel, and NonDIntegration::numIntegrations.

14.150.3.2 void print_points_weights (const String & *tabular_name*) [protected]

output integration points and weights to a tabular file

```
Virtual function called from probDescDB-based constructors and from
NonDIntegration::core_run()
```

void NonDIntegration:: check_variables(const std::vector<Pecos::RandomVariable>& x_ran_vars) { base class default definition of virtual function bool err_flag = false;

numContDesVars = numContIntervalVars = numContStateVars = 0; size_t i, num_v = x_ran_vars.size(); short x_type; for (i=0; i<num_v; ++i) { x_type = x_ran_vars[i].type(); if (x_type == Pecos::CONTINUOUS_DESIGN) ++numContDesVars; else if (x_type == Pecos::CONTINUOUS_INTERVAL) ++numContIntervalVars; else if (x_type == Pecos::CONTINUOUS_STATE) ++numContStateVars; }

if (x_ran_vars.size() != numContinuousVars || numContEpistUncVars != numContIntervalVars || numContinuousVars != numContDesVars + numContAleatUncVars + numContEpistUncVars + numContStateVars) { Cerr << "Error: mismatch in active variable counts in NonDIntegration::" << "check_variables()." << std::endl; err_flag = true; }

if (err_flag) abort_handler(-1); }

References Analyzer::allSamples, Model::continuous_variable_labels(), Iterator::iteratedModel, NonDIntegration::numIntDriver, and Dakota::write_precision.

Referenced by NonDCubature::get_parameter_sets(), NonDQuadrature::get_parameter_sets(), and NonDSparseGrid::get_parameter_sets().

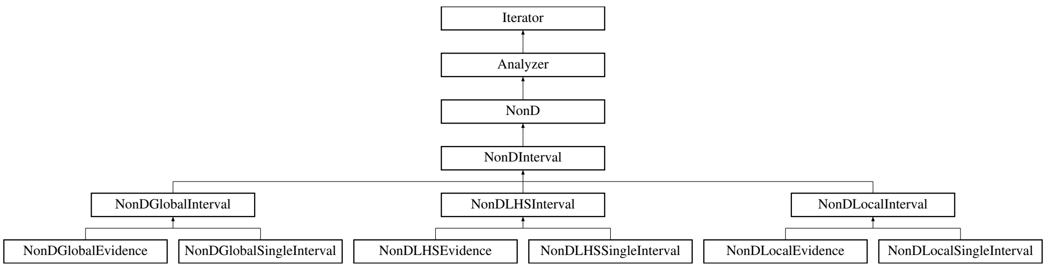
The documentation for this class was generated from the following files:

- NonDIntegration.hpp
- NonDIntegration.cpp

14.151 NonDInterval Class Reference

Base class for interval-based methods within DAKOTA/UQ.

Inheritance diagram for NonDInterval:



Public Member Functions

- NonDInterval (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDInterval ()

  destructor
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the cumulative distribution functions for belief and plausibility
- bool resize ()

  reinitializes iterator based on new variable size

Protected Member Functions

- void initialize_final_statistics ()

  initialize finalStatistics for belief/plausibility results sets
- void compute_evidence_statistics ()

  method for computing belief and plausibility values for response levels or vice-versa

- void calculate_cells_and_bpas ()

  computes the interval combinations (cells) and their bpas replaces CBPIIC_F77 from wrapper calculate_basic_prob-_intervals()
- void calculate_cbf_cpf (bool complementary=true)

  function to compute (complementary) distribution functions on belief and plausibility replaces CCBFPF_F77 from wrapper calculate_cum_belief_plaus()

Protected Attributes

- size_t numContIntervalVars

  number of variables of type CONTINUOUS_INTERVAL_UNCERTAIN
- size_t numDiscIntervalVars

  number of variables of type DISCRETE_INTERVAL_UNCERTAIN
- size_t numDiscSetIntUncVars

  number of variables of type DISCRETE_UNCERTAIN_SET_INT
- size_t numDiscSetRealUncVars

  number of variables of type DISCRETE_UNCERTAIN_SET_REAL
- bool singleIntervalFlag

  flag for SingleInterval derived class
- RealVectorArray ccBelFn

  Storage array to hold CCBF values.
- RealVectorArray ccPlausFn

  Storage array to hold CCPF values.
- RealVectorArray ccBelVal

  Storage array to hold CCB response values.
- RealVectorArray ccPlausVal

  Storage array to hold CCP response values.
- RealVectorArray cellContLowerBounds

  Storage array to hold cell lower bounds for continuous variables.
- RealVectorArray cellContUpperBounds

  Storage array to hold cell upper bounds for continuous variables.
- IntVectorArray cellIntRangeLowerBounds

  Storage array to hold cell lower bounds for discrete int range variables.
- IntVectorArray cellIntRangeUpperBounds

  Storage array to hold cell upper bounds for discrete int range variables.
- IntVectorArray cellIntSetBounds

  Storage array to hold cell values for discrete integer set variables.
- IntVectorArray cellRealSetBounds

  Storage array to hold cell value for discrete real set variables.
- RealVectorArray cellFnLowerBounds

  Storage array to hold cell min.
- RealVectorArray cellFnUpperBounds

  Storage array to hold cell max.
- RealVector cellBPA

  Storage array to hold cell bpa.
- size_t respFnCntr

  response function counter
- size_t cellCntr

  cell counter
- size_t numCells

  total number of interval combinations

Additional Inherited Members

14.151.1 Detailed Description

Base class for interval-based methods within DAKOTA/UQ.

The NonDInterval class implements the propagation of epistemic uncertainty using either pure interval propagation or Dempster-Shafer theory of evidence. In the latter approach, one assigns a set of basic probability assignments (BPA) to intervals defined for the uncertain variables. Input interval combinations are calculated, along with their BPA. Currently, the response function is evaluated at a set of sample points, then a response surface is constructed which is sampled extensively to find the minimum and maximum within each input interval cell, corresponding to the belief and plausibility within that cell, respectively. This data is then aggregated to calculate cumulative distribution functions for belief and plausibility.

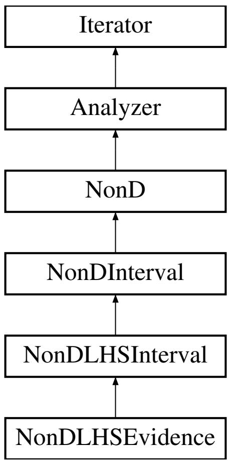
The documentation for this class was generated from the following files:

- NonDInterval.hpp
- NonDInterval.cpp

14.152 NonDLHSEvidence Class Reference

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

Inheritance diagram for NonDLHSEvidence:



Public Member Functions

- NonDLHSEvidence (ProblemDescDB &problem_db, Model &model)

    constructor
- ∼NonDLHSEvidence ()

    destructor
- void initialize ()

    perform any required initialization
- void post_process_samples ()

    post-process the output from executing lhsSampler

Additional Inherited Members

14.152.1 Detailed Description

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

The NonDEvidence class implements the propagation of epistemic uncertainty using Dempster-Shafer theory of evidence. In this approach, one assigns a set of basic probability assignments (BPA) to intervals defined for the uncertain variables. Input interval combinations are calculated, along with their BPA. Currently, the response function is evaluated at a set of sample points, then a response surface is constructed which is sampled extensively to find the minimum and maximum within each input interval cell, corresponding to the belief and plausibility within that cell, respectively. This data is then aggregated to calculate cumulative distribution functions for belief and plausibility.

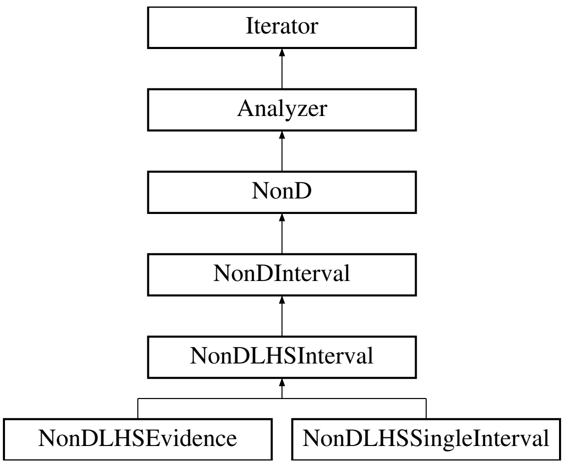
The documentation for this class was generated from the following files:

- NonDLHSEvidence.hpp
- NonDLHSEvidence.cpp

14.153 NonDLHSInterval Class Reference

Class for the LHS-based interval methods within DAKOTA/UQ.

Inheritance diagram for NonDLHSInterval:



Public Member Functions

- NonDLHSInterval (ProblemDescDB &problem_db, Model &model)

    constructor
- ∼NonDLHSInterval ()

    destructor
- void derived_init_communicators (ParLevLIter pl_iter)

    derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

    derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

    derived class contributions to freeing the communicators associated with this Iterator instance
- void core_run ()

    performs an epistemic uncertainty propagation using LHS samples

Protected Member Functions

- virtual void initialize ()

    perform any required initialization
- virtual void post_process_samples ()=0

    post-process the output from executing lhsSampler

Protected Attributes

- Iterator lhsSampler

    the LHS sampler instance
- const int seedSpec

    the user seed specification (default is 0)
- int numSamples

    the number of samples used
- String rngName

    name of the random number generator

Additional Inherited Members

14.153.1 Detailed Description

Class for the LHS-based interval methods within DAKOTA/UQ.

The NonDLHSInterval class implements the propagation of epistemic uncertainty using LHS-based methods.

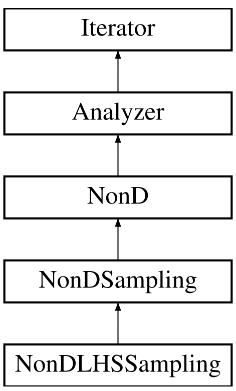
The documentation for this class was generated from the following files:

- NonDLHSInterval.hpp
- NonDLHSInterval.cpp

14.154 NonDLHSSampling Class Reference

Performs LHS and Monte Carlo sampling for uncertainty quantification.

Inheritance diagram for NonDLHSSampling:



Public Member Functions

- NonDLHSSampling (ProblemDescDB &problem_db, Model &model)
    standard constructor
- NonDLHSSampling (Model &model, unsigned short sample_type, int samples, int seed, const String &rng, bool vary_pattern=true, short sampling_vars_mode=ACTIVE)
    alternate constructor for sample generation and evaluation "on the fly"
- NonDLHSSampling (unsigned short sample_type, int samples, int seed, const String &rng, const RealVector &lower_bnds, const RealVector &upper_bnds)
    alternate constructor for uniform sample generation "on the fly"
- NonDLHSSampling (unsigned short sample_type, int samples, int seed, const String &rng, const RealVector &means, const RealVector &std_devs, const RealVector &lower_bnds, const RealVector &upper_bnds, RealSymMatrix &correl)
    alternate constructor for sample generation of correlated normals "on the fly"
- ∼NonDLHSSampling ()
    destructor

Protected Member Functions

- void sampling_increment ()
    increment to next in sequence of refinement samples
- void pre_run ()
    generate LHS samples in non-VBD cases
- void core_run ()
    perform the evaluate parameter sets portion of run
- void post_run (std::ostream &s)
    generate statistics for LHS runs in non-VBD cases
- void post_input ()
    read tabular data for post-run mode
- void update_final_statistics ()
    update finalStatistics and (if MC sampling) finalStatErrors
- void compute_pca (std::ostream &s)
    compute a principal components analysis on the sample set
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)
    print the final statistics
- void d_optimal_parameter_set (int previous_samples, int new_samples, RealMatrix &full_samples)
    generate a d-optimal parameter set, leaving the first previous_samples columns intact and adding new_samples new columns following them
- void initial_increm_lhs_set (int new_samples, RealMatrix &full_samples, IntMatrix &full_ranks)
    Populate the first new_samples columns of allSamples with an LHS design and update the stored ranks.
- void increm_lhs_parameter_set (int previous_samples, int new_samples, RealMatrix &full_samples, IntMatrix &all_ranks)
    generate a new batch that is Latin w.r.t. the previous samples
- void store_ranks (const RealMatrix &sample_values, IntMatrix &sample_ranks)
    store the ranks of the last generated sample for continuous (based on sampleRanks) and calculate/store discrete ranks
- void store_ranks (IntMatrix &full_ranks)
    store the combined ranks from sampleRanks to leading submatrix local cached ranks matrix
- void combine_discrete_ranks (const RealMatrix &initial_values, const RealMatrix &increm_values)
    merge the discrete ranks into a submatrix of sampleRanks
- void print_header_and_statistics (std::ostream &s, const int &num_samples)
    Print a header and summary statistics.

- void archive_results (int num_samples, size_t ind_inc=0)

  Archive all results.
- void store_evaluations ()

  Store samples in a matrix for bootstrapping.
- Real **bootstrap_covariance** (const size_t qoi)

Static Protected Member Functions

- static bool rank_sort (const int &x, const int &y)

  sort algorithm to compute ranks for rank correlations

Private Attributes

- size_t numResponseFunctions

  number of response functions; used to distinguish NonD from opt/NLS usage
- IntVector refineSamples

  list of refinement sample batch sizes
- bool dOptimal

  whether to generate d-optimal point sets
- size_t numCandidateDesigns

  number of candidate designs to generate for classical D-optimal designs
- Real oversampleRatio

  oversampling ratio for Leja D-optimal candidate set generation
- bool varBasedDecompFlag

  flags computation of variance-based decomposition indices
- bool pcaFlag

  flag to specify the calculation of principal components
- Real percentVarianceExplained

  Threshold to keep number of principal components that explain this much variance.
- RealMatrix qoiSamplesMatrix

  Datastructure to store samples which can be used for bootstrapping.

Static Private Attributes

- static RealArray rawData

  static data used by static rank_sort() fn

Additional Inherited Members

14.154.1 Detailed Description

Performs LHS and Monte Carlo sampling for uncertainty quantification.

The Latin Hypercube Sampling (LHS) package from Sandia Albuquerque's Risk and Reliability organization provides comprehensive capabilities for Monte Carlo and Latin Hypercube sampling within a broad array of user-specified probabilistic parameter distributions. It enforces user-specified rank correlations through use of a mixing routine. The NonDLHSSampling class provides a C++ wrapper for the LHS library and is used for performing forward propagations of parameter uncertainties into response statistics.

Batch generation options, including D-Optimal and incremental LHS are provided.

The incremental LHS sampling capability allows one to supplement an initial sample of size n to size 2n while maintaining the correct stratification of the 2n samples and also maintaining the specified correlation structure. The incremental version of LHS will return a sample of size n, which when combined with the original sample of size n, allows one to double the size of the sample.

14.154.2 Constructor & Destructor Documentation

14.154.2.1 NonDLHSSampling (ProblemDescDB & *problem_db*, Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), SharedVariablesData::active_components_totals(), Model::current_-variables(), NonDLHSSampling::dOptimal, NonD::initialize_final_statistics(), Model::num_primary_fns(), NonD-LHSSampling::numCandidateDesigns, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer-::numDiscreteStringVars, Analyzer::numFunctions, NonDLHSSampling::numResponseFunctions, Iterator::output-Level, NonDLHSSampling::oversampleRatio, Model::primary_fn_type(), NonDLHSSampling::qoiSamplesMatrix, NonDLHSSampling::refineSamples, NonDSampling::sampleType, Variables::shared_data(), and Dakota::svd().

14.154.2.2 NonDLHSSampling (Model & *model*, unsigned short *sample_type*, int *samples*, int *seed*, const String & *rng*, bool *vary_pattern* = `true`, short *sampling_vars_mode* = `ACTIVE`)

alternate constructor for sample generation and evaluation "on the fly"

This alternate constructor is used for generation and evaluation of Model-based sample sets. A set_db_list_nodes has not been performed so required data must be passed through the constructor. It's purpose is to avoid the need for a separate LHS specification within methods that use LHS sampling.

14.154.2.3 NonDLHSSampling (unsigned short *sample_type*, int *samples*, int *seed*, const String & *rng*, const RealVector & *lower_bnds*, const RealVector & *upper_bnds*)

alternate constructor for uniform sample generation "on the fly"

This alternate constructor is used by ConcurrentStrategy for generation of uniform, uncorrelated sample sets. It is *not* a letter-envelope instantiation and a set_db_list_nodes has not been performed. It is called with all needed data passed through the constructor and is designed to allow more flexibility in variables set definition (i.e., relax connection to a variables specification and allow sampling over parameter sets such as multiobjective weights). In this case, a Model is not used and the object must only be used for sample generation (no evaluation).

References NonDSampling::get_parameter_sets().

14.154.2.4 NonDLHSSampling (unsigned short *sample_type*, int *samples*, int *seed*, const String & *rng*, const RealVector & *means*, const RealVector & *std_devs*, const RealVector & *lower_bnds*, const RealVector & *upper_bnds*, RealSymMatrix & *correl*)

alternate constructor for sample generation of correlated normals "on the fly"

This alternate constructor is used to generate correlated normal sample sets. It is *not* a letter-envelope instantiation and a set_db_list_nodes has not been performed. It is called with all needed data passed through the constructor. In this case, a Model is not used and the object must only be used for sample generation (no evaluation).

References NonDSampling::get_parameter_sets().

14.154.3 Member Function Documentation

14.154.3.1 void core_run ( ) `[protected]`, `[virtual]`

perform the evaluate parameter sets portion of run

Loop over the set of samples and compute responses. Compute statistics on the set of responses if statsFlag is set.

Reimplemented from Iterator.

References NonDSampling::allDataFlag, Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, NonDLHS-Sampling::numResponseFunctions, and NonDSampling::statsFlag.

14.154.3.2 void d_optimal_parameter_set (int *previous_samples,* int *new_samples,* RealMatrix & *full_samples*) [protected]

generate a d-optimal parameter set, leaving the first previous_samples columns intact and adding new_samples new columns following them

For now, when this function is called, numSamples is the number of new samples to generate.

References Model::current_variables(), Dakota::det_AtransA(), NonDSampling::get_parameter_sets(), Probability-TransformModel::initialize_distribution_types(), Iterator::iteratedModel, NonDSampling::mode_counts(), Model-::multivariate_distribution(), NonDLHSSampling::numCandidateDesigns, Iterator::outputLevel, NonDLHSSampling-::oversampleRatio, and NonDSampling::transform_samples().

Referenced by NonDLHSSampling::pre_run().

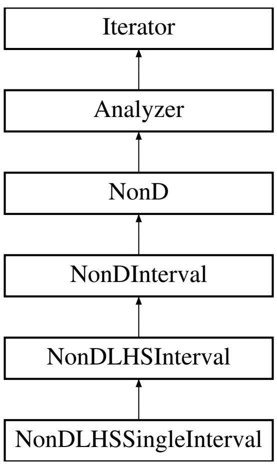
The documentation for this class was generated from the following files:

- NonDLHSSampling.hpp
- NonDLHSSampling.cpp

14.155 NonDLHSSingleInterval Class Reference

Class for pure interval propagation using LHS.

Inheritance diagram for NonDLHSSingleInterval:



Public Member Functions

- NonDLHSSingleInterval (ProblemDescDB &problem_db, Model &model)

    constructor
- ∼NonDLHSSingleInterval ()

    destructor

Protected Member Functions

- void initialize ()

  perform any required initialization
- void post_process_samples ()

  post-process the output from executing lhsSampler

Private Attributes

- size_t statCntr

  counter for finalStatistics

Additional Inherited Members

14.155.1 Detailed Description

Class for pure interval propagation using LHS.

The NonDSingleInterval class implements the propagation of epistemic uncertainty using ...

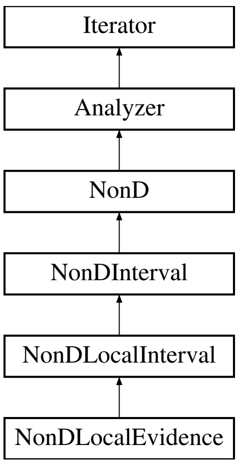
The documentation for this class was generated from the following files:

- NonDLHSSingleInterval.hpp
- NonDLHSSingleInterval.cpp

14.156 NonDLocalEvidence Class Reference

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

Inheritance diagram for NonDLocalEvidence:



Public Member Functions

- NonDLocalEvidence (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDLocalEvidence ()

  destructor

Protected Member Functions

- void initialize ()

    perform any required initialization
- void set_cell_bounds ()

    set the optimization variable bounds for each cell
- void truncate_to_cell_bounds (RealVector &initial_pt)

    truncate initial_pt to respect current cell lower/upper bounds
- void post_process_cell_results (bool maximize)

    post-process a cell minimization/maximization result
- void post_process_response_fn_results ()

    post-process the interval computed for a response function
- void post_process_final_results ()

    perform final post-processing

Additional Inherited Members

14.156.1 Detailed Description

Class for the Dempster-Shafer Evidence Theory methods within DAKOTA/UQ.

The NonDEvidence class implements the propagation of epistemic uncertainty using Dempster-Shafer theory of evidence. In this approach, one assigns a set of basic probability assignments (BPA) to intervals defined for the uncertain variables. Input interval combinations are calculated, along with their BPA. Currently, the response function is evaluated at a set of sample points, then a response surface is constructed which is sampled extensively to find the minimum and maximum within each input interval cell, corresponding to the belief and plausibility within that cell, respectively. This data is then aggregated to calculate cumulative distribution functions for belief and plausibility.

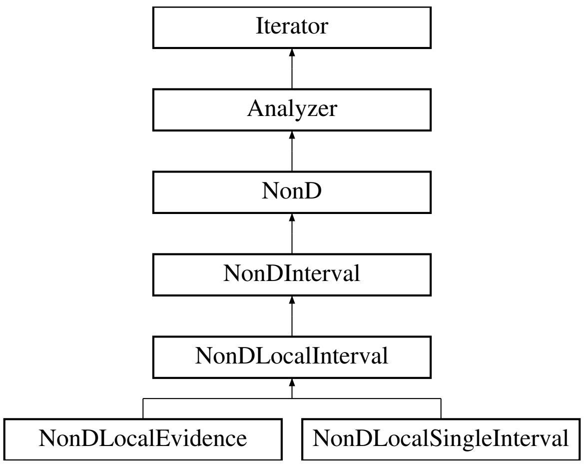
The documentation for this class was generated from the following files:

- NonDLocalEvidence.hpp
- NonDLocalEvidence.cpp

14.157 NonDLocalInterval Class Reference

Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

Inheritance diagram for NonDLocalInterval:



Public Member Functions

- NonDLocalInterval (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDLocalInterval ()

  destructor
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- void core_run ()

  Performs a gradient-based optimization to determine interval bounds for an entire function or interval bounds on a particular statistical estimator.
- void check_sub_iterator_conflict ()

  detect any conflicts due to recursive use of the same Fortran solver
- unsigned short uses_method () const

  return name of any enabling iterator used by this iterator
- void method_recourse ()

  perform a method switch, if possible, due to a detected conflict

Protected Member Functions

- virtual void initialize ()

  perform any required initialization
- virtual void set_cell_bounds ()

  set the optimization variable bounds for each cell
- virtual void truncate_to_cell_bounds (RealVector &initial_pt)

  truncate initial_pt to respect current cell lower/upper bounds
- virtual void post_process_cell_results (bool maximize)

  post-process a cell minimization/maximization result
- virtual void post_process_response_fn_results ()

  post-process the interval computed for a response function
- virtual void post_process_final_results ()

  perform final post-processing

Protected Attributes

- Iterator minMaxOptimizer

  local gradient-based optimizer
- Model minMaxModel

  recast model which extracts the active objective function

Static Private Member Functions

- static void extract_objective (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used to extract the active objective function when optimizing for an interval lower or upper bound

Private Attributes

- bool npsolFlag

  flag representing the gradient-based optimization algorithm selection (NPSOL SQP or OPT++ NIP)

Static Private Attributes

- static NonDLocalInterval ∗ nondLIInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

14.157.1 Detailed Description

Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

The NonDLocalInterval class supports local gradient-based optimization apporaches to determining interval bounds for epistemic UQ. The interval bounds may be on the entire function in the case of pure interval analysis (e.g. intervals on input = intervals on output), or the intervals may be on statistics of an "inner loop" aleatory analysis such as intervals on means, variances, or percentile levels.

14.157.2 Member Function Documentation

14.157.2.1 void check_sub_iterator_conflict ( ) [virtual]

detect any conflicts due to recursive use of the same Fortran solver

This is used to avoid clashes in state between non-object-oriented (i.e., F77, C) iterator executions, when such iterators could potentially be executing simultaneously (e.g., nested execution). It is not an issue (and a used method is not reported) in cases where a helper execution is completed before a lower level one could be initiated; an example of this is DIRECT for maximization of expected improvement: the EIF maximization is completed before a new point evaluation (which could include nested iteration) is performed.

Reimplemented from Iterator.

References Iterator::is_null(), Iterator::iteratedModel, Iterator::method_name(), Iterator::method_recourse(), NonDLocalInterval::npsolFlag, Model::subordinate_iterator(), Model::subordinate_models(), and Iterator::uses_method().

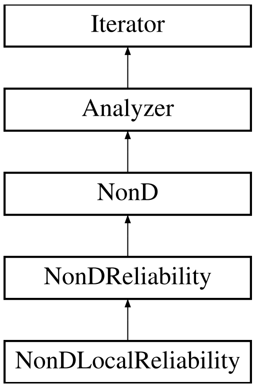
The documentation for this class was generated from the following files:

- NonDLocalInterval.hpp
- NonDLocalInterval.cpp

14.158 NonDLocalReliability Class Reference

Class for the reliability methods within DAKOTA/UQ.

Inheritance diagram for NonDLocalReliability:



Public Member Functions

- NonDLocalReliability (ProblemDescDB &problem_db, Model &model)

    constructor
- ∼NonDLocalReliability ()

    destructor
- void derived_init_communicators (ParLevLIter pl_iter)

    derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

    derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

    derived class contributions to freeing the communicators associated with this Iterator instance
- void initialize_graphics (int iterator_server_id=1)

    initialize graphics customized for local reliability methods
- void pre_run ()

    pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()

    core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

    print the final iterator results
- void check_sub_iterator_conflict ()

    detect any conflicts due to recursive use of the same Fortran solver
- unsigned short uses_method () const

    return name of any enabling iterator used by this iterator
- void method_recourse ()

    perform a method switch, if possible, due to a detected conflict

Private Member Functions

- void initial_taylor_series ()

    convenience function for performing the initial limit state Taylor-series approximation
- void mean_value ()

    convenience function for encapsulating the simple Mean Value computation of approximate statistics and importance factors
- void mpp_search ()

    convenience function for encapsulating the reliability methods that employ a search for the most probable point (AMV, AMV+, FORM, SORM)
- void initialize_class_data ()

convenience function for initializing class scope arrays

- void initialize_level_data ()

  convenience function for initializing/warm starting MPP search data for each response function prior to level 0

- void initialize_mpp_search_data ()

  convenience function for initializing/warm starting MPP search data for each z/p/beta level for each response function

- void update_mpp_search_data (const Variables &vars_star, const Response &resp_star)

  convenience function for updating MPP search data for each z/p/beta level for each response function

- void update_level_data ()

  convenience function for updating z/p/beta level data and final statistics following MPP convergence

- void update_pma_maximize (const RealVector &mpp_u, const RealVector &fn_grad_u, const RealSymMatrix &fn_hess_u)

  update pmaMaximizeG from prescribed probabilities or prescribed generalized reliabilities by inverting second-order integrations

- void update_limit_state_surrogate ()

  convenience function for passing the latest variables/response data to the data fit embedded within uSpaceModel

- void assign_mean_data ()

  update mostProbPointX/U, computedRespLevel, fnGradX/U, and fnHessX/U from ranVarMeansX/U, fnValsMeanX, fnGradsMeanX, and fnHessiansMeanX

- void dg_ds_eval (const RealVector &x_vars, const RealVector &fn_grad_x, RealVector &final_stat_grad)

  convenience function for evaluating dg/ds

- Real dp2_dbeta_factor (Real beta, bool cdf_flag)

  compute factor for derivative of second-order probability with respect to reliability index (from differentiating BREITU-NG or HOHENRACK expressions)

- void truth_evaluation (short mode)

  perform an evaluation of the actual model and store value,grad,Hessian data in X,U spaces

- Real signed_norm (const RealVector &mpp_u, const RealVector &fn_grad_u, bool cdf_flag)

  convert norm of mpp_u (u-space solution) to a signed reliability index

- Real signed_norm (Real norm_mpp_u)

  convert norm of u-space vector to a signed reliability index

- Real signed_norm (Real norm_mpp_u, const RealVector &mpp_u, const RealVector &fn_grad_u, bool cdf_-flag)

  shared helper function

- Real probability (Real beta)

  Convert reliability to probability using a first-order integration.

- Real probability (bool cdf_flag, const RealVector &mpp_u, const RealVector &fn_grad_u, const RealSym-Matrix &fn_hess_u)

  Convert computed reliability to probability using either a first-order or second-order integration.

- Real probability (Real beta, bool cdf_flag, const RealVector &mpp_u, const RealVector &fn_grad_u, const RealSymMatrix &fn_hess_u)

  Convert provided reliability to probability using either a first-order or second-order integration.

- Real reliability (Real p)

  Convert probability to reliability using the inverse of a first-order integration.

- Real reliability (Real p, bool cdf_flag, const RealVector &mpp_u, const RealVector &fn_grad_u, const Real-SymMatrix &fn_hess_u)

  Convert probability to reliability using the inverse of a first-order or second-order integration.

- bool reliability_residual (const Real &p, const Real &beta, const RealVector &kappa, Real &res)

  compute the residual for inversion of second-order probability corrections using Newton's method (called by reliabil-ity(p))

- Real reliability_residual_derivative (const Real &p, const Real &beta, const RealVector &kappa)

  compute the residual derivative for inversion of second-order probability corrections using Newton's method (called by reliability(p))

- void principal_curvatures (const RealVector &mpp_u, const RealVector &fn_grad_u, const RealSymMatrix &fn_hess_u, RealVector &kappa_u)

Compute the kappaU vector of principal curvatures from fnHessU.
- void scale_curvature (Real beta, bool cdf_flag, const RealVector &kappa, RealVector &scaled_kappa)

  scale copy of principal curvatures by -1 if needed; else take a view

Static Private Member Functions

- static void RIA_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the objective function in the Reliability Index Approach (RIA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the objective function of (norm u)^2.
- static void RIA_constraint_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the constraint function in the Reliability Index Approach (RIA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the constraint of G(u) = response level.
- static void PMA_objective_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the objective function in the Performance Measure Approach (PMA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the objective function of G(u).
- static void PMA_constraint_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the constraint function in the first-order Performance Measure Approach (PMA) problem formulation. This optimization problem performs the search for the most probable point (MPP) with the equality constraint of (norm u)^2 = (beta-bar)^2.
- static void PMA2_constraint_eval (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

  static function used as the constraint function in the second-order Performance Measure Approach (PMA) problem formulation. This optimization problem performs the search for the most probable point (MPP) with the equality constraint of beta = beta*-bar.*
- static void PMA2_set_mapping (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)

  static function used to augment the sub-model ASV requests for second-order PMA

Private Attributes

- Real computedRespLevel

  output response level calculated
- Real computedRelLevel

  output reliability level calculated for RIA and 1st-order PMA
- Real computedGenRelLevel

  output generalized reliability level calculated for 2nd-order PMA
- RealVector fnGradX

  actual x-space gradient for current function from most recent response evaluation
- RealVector fnGradU

  u-space gradient for current function updated from fnGradX and Jacobian dx/du
- RealSymMatrix fnHessX

  actual x-space Hessian for current function from most recent response evaluation
- RealSymMatrix fnHessU

  u-space Hessian for current function updated from fnHessX and Jacobian dx/du
- RealVector kappaU

  principal curvatures derived from eigenvalues of orthonormal transformation of fnHessU

- RealVector fnValsMeanX

  response function values evaluated at mean x
- RealMatrix fnGradsMeanX

  response function gradients evaluated at mean x
- RealSymMatrixArray fnHessiansMeanX

  response function Hessians evaluated at mean x
- RealVector ranVarMeansX

  vector of means for all uncertain random variables in x-space
- RealVector ranVarStdDevsX

  vector of std deviations for all uncertain random variables in x-space
- RealVector ranVarMeansU

  vector of means for all uncertain random variables in u-space
- bool initialPtUserSpec

  flag indicating user specification of (any portion of) initialPtU
- RealVector initialPtUSpec

  user specification or default initial guess for local optimization
- RealVector initialPtU

  current starting point for MPP searches in u-space
- RealVector mostProbPointX

  location of MPP in x-space
- RealVector mostProbPointU

  location of MPP in u-space
- RealVectorArray prevMPPULev0

  array of converged MPP's in u-space for level 0. Used for warm-starting initialPtU within RBDO.
- RealMatrix prevFnGradDLev0

  matrix of limit state sensitivities w.r.t. inactive/design variables for level 0. Used for warm-starting initialPtU within RBDO.
- RealMatrix prevFnGradULev0

  matrix of limit state sensitivities w.r.t. active/uncertain variables for level 0. Used for warm-starting initialPtU within RBDO.
- RealVector prevICVars

  previous design vector. Used for warm-starting initialPtU within RBDO.
- ShortArray prevCumASVLev0

  accumulation (using |=) of all previous design ASV's from requested finalStatistics. Used to detect availability of prevFnGradDLev0 data for warm-starting initialPtU within RBDO.
- bool npsolFlag

  flag representing the optimization MPP search algorithm selection (NPSOL SQP or OPT++ NIP)
- bool warmStartFlag

  flag indicating the use of warm starts
- bool nipModeOverrideFlag

  flag indicating the use of move overrides within OPT++ NIP
- bool curvatureDataAvailable

  flag indicating that sufficient data (i.e., fnGradU, fnHessU, mostProbPointU) is available for computing principal curvatures
- bool kappaUpdated

  track when kappaU requires updating via principal_curvatures()
- short integrationOrder

  integration order (1 or 2) provided by `integration` *specification*
- short secondOrderIntType

  type of second-order integration: Breitung, Hohenbichler-Rackwitz, or Hong
- Real curvatureThresh

cut-off value for 1/sqrt() term in second-order probability corrections.

- short taylorOrder

  order of Taylor series approximations (1 or 2) in MV/AMV/AMV+ derived from hessian type

- RealMatrix impFactor

  importance factors predicted by MV

- int npsolDerivLevel

  derivative level for NPSOL executions (1 = analytic grads of objective fn, 2 = analytic grads of constraints, 3 = analytic grads of both).

- unsigned short warningBits

  set of warnings accumulated during execution

Static Private Attributes

- static NonDLocalReliability ∗ nondLocRelInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

14.158.1 Detailed Description

Class for the reliability methods within DAKOTA/UQ.

The NonDLocalReliability class implements the following reliability methods through the support of different limit state approximation and integration options: mean value (MVFOSM/MVSOSM), advanced mean value method (AMV, AMV^2) in x- or u-space, iterated advanced mean value method (AMV+, AMV^2+) in x- or u-space, two-point adaptive nonlinearity approximation (TANA) in x- or u-space, first order reliability method (FORM), and second order reliability method (SORM). All options except mean value employ an optimizer (currently NPSOL SQP or OPT++ NIP) to solve an equality-constrained optimization problem for the most probable point (MPP). The MPP search may be formulated as the reliability index approach (RIA) for mapping response levels to reliabilities/probabilities or as the performance measure approach (PMA) for performing the inverse mapping of reliability/probability levels to response levels.

14.158.2 Member Function Documentation

14.158.2.1 void pre_run ( ) [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

References Model::initialize_mapping(), Iterator::methodPCIter, NonD::miPLIndex, NonDReliability::mppModel, NonDReliability::mppSearchType, Analyzer::pre_run(), and Model::update_from_subordinate_model().

14.158.2.2 void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References NonD::compute_densities(), NonDReliability::importanceSampler, NonDReliability::integrationRefinement, Iterator::iterator_rep(), NonDLocalReliability::mean_value(), NonDLocalReliability::mpp_search(), NonDReliability::mppSearchType, NonD::pdfOutput, and NonD::resize_final_statistics_gradients().

14.158.2.3 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

References NonD::cdfFlag, NonD::computedGenRelLevels, NonD::computedProbLevels, NonD::computedRelLevels, NonD::computedRespLevels, Model::continuous_variable_labels(), NonD::finalMomentsType, NonDLocalReliability::impFactor, Iterator::iteratedModel, NonD::momentStats, NonDReliability::mppSearchType, Model::multivariate_distribution(), Analyzer::numContinuousVars, Analyzer::numFunctions, NonD::print_densities(), Model::response_labels(), NonDLocalReliability::warningBits, and Dakota::write_precision.

14.158.2.4 void check_sub_iterator_conflict ( ) [virtual]

detect any conflicts due to recursive use of the same Fortran solver

This is used to avoid clashes in state between non-object-oriented (i.e., F77, C) iterator executions, when such iterators could potentially be executing simultaneously (e.g., nested execution). It is not an issue (and a used method is not reported) in cases where a helper execution is completed before a lower level one could be initiated; an example of this is DIRECT for maximization of expected improvement: the EIF maximization is completed before a new point evaluation (which could include nested iteration) is performed.

Reimplemented from Iterator.

References Iterator::is_null(), Iterator::iteratedModel, Iterator::method_name(), Iterator::method_recourse(), NonDReliability::mppSearchType, NonDLocalReliability::npsolFlag, Model::subordinate_iterator(), Model::subordinate_models(), and Iterator::uses_method().

14.158.2.5 void RIA_objective_eval (const Variables & *sub_model_vars*, const Variables & *recast_vars*, const Response & *sub_model_response*, Response & *recast_response*) [static], [private]

static function used as the objective function in the Reliability Index Approach (RIA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the objective function of (norm u)^2.

This function recasts a G(u) response set (already transformed and approximated in other recursions) into an RIA objective function.

References Response::active_set_request_vector(), Variables::continuous_variables(), Response::function_gradient_view(), Response::function_hessian_view(), and Response::function_value().

Referenced by NonDLocalReliability::mpp_search().

14.158.2.6 void RIA_constraint_eval (const Variables & *sub_model_vars*, const Variables & *recast_vars*, const Response & *sub_model_response*, Response & *recast_response*) [static], [private]

static function used as the constraint function in the Reliability Index Approach (RIA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the constraint of G(u) = response level.

This function recasts a G(u) response set (already transformed and approximated in other recursions) into an RIA equality constraint.

References Response::active_set_request_vector(), Response::function_gradient(), Response::function_gradient-_view(), Response::function_hessian(), Response::function_value(), NonDLocalReliability::nondLocRelInstance, NonDReliability::requestedTargetLevel, and NonDReliability::respFnCount.

Referenced by NonDLocalReliability::mpp_search().

14.158.2.7 void PMA_objective_eval (const Variables & *sub_model_vars,* const Variables & *recast_vars,* const Response & *sub_model_response,* Response & *recast_response*) [static], [private]

static function used as the objective function in the Performance Measure Approach (PMA) problem formulation. This equality-constrained optimization problem performs the search for the most probable point (MPP) with the objective function of G(u).

This function recasts a G(u) response set (already transformed and approximated in other recursions) into an PMA objective function.

References Response::active_set_request_vector(), Variables::continuous_variables(), NonDLocalReliability-::curvatureDataAvailable, Response::function_gradient(), Response::function_gradient_view(), Response::function-_hessian(), Response::function_hessian_view(), Response::function_value(), NonDLocalReliability::integration-Order, NonDLocalReliability::kappaUpdated, NonDReliability::mppSearchType, NonDLocalReliability::nondLocRel-Instance, NonDReliability::pmaMaximizeG, NonDReliability::respFnCount, and NonDLocalReliability::update_pma-_maximize().

Referenced by NonDLocalReliability::mpp_search().

14.158.2.8 void PMA_constraint_eval (const Variables & *sub_model_vars,* const Variables & *recast_vars,* const Response & *sub_model_response,* Response & *recast_response*) [static], [private]

static function used as the constraint function in the first-order Performance Measure Approach (PMA) problem formulation. This optimization problem performs the search for the most probable point (MPP) with the equality constraint of (norm u)^2 = (beta-bar)^2.

This function recasts a G(u) response set (already transformed and approximated in other recursions) into a first-order PMA equality constraint on reliability index beta.

References Response::active_set_request_vector(), Variables::continuous_variables(), Response::function_-gradient_view(), Response::function_hessian_view(), Response::function_value(), NonDLocalReliability::nond-LocRelInstance, and NonDReliability::requestedTargetLevel.

Referenced by NonDLocalReliability::mpp_search().

14.158.2.9 void PMA2_constraint_eval (const Variables & *sub_model_vars,* const Variables & *recast_vars,* const Response & *sub_model_response,* Response & *recast_response*) [static], [private]

static function used as the constraint function in the second-order Performance Measure Approach (PMA) problem formulation. This optimization problem performs the search for the most probable point (MPP) with the equality constraint of beta∗ = beta∗-bar.

This function recasts a G(u) response set (already transformed and approximated in other recursions) into a second-order PMA equality constraint on generalized reliability index beta-star.

References Dakota::abort_handler(), Response::active_set_request_vector(), NonD::cdfFlag, NonDLocal-Reliability::computedGenRelLevel, NonDLocalReliability::computedRelLevel, Variables::continuous_variables(), NonDLocalReliability::dp2_dbeta_factor(), NonDLocalReliability::fnGradU, NonDLocalReliability::fnHessU, Response::function_gradient_view(), Response::function_hessian(), Response::function_value(), NonDLocal-Reliability::mostProbPointU, NonDReliability::mppSearchType, NonDLocalReliability::nondLocRelInstance, Non-DLocalReliability::probability(), NonDLocalReliability::reliability(), NonDReliability::requestedTargetLevel, NonD-Reliability::respFnCount, and NonDLocalReliability::signed_norm().

Referenced by NonDLocalReliability::mpp_search().

14.158.2.10 void initial_taylor_series ( ) [private]

convenience function for performing the initial limit state Taylor-series approximation

An initial first- or second-order Taylor-series approximation is required for MV/AMV/AMV+/TANA or for the case where momentStats (from MV) are required within finalStatistics for subIterator usage of NonDLocalReliability.

References Response::active_set_request_vector(), Iterator::activeSet, Model::component_parallel_mode(), Model::continuous_variables(), Model::current_response(), Model::evaluate(), NonD::finalMomentsType, NonD::finalStatistics, NonDLocalReliability::fnGradsMeanX, NonDLocalReliability::fnHessiansMeanX, NonDLocalReliability::fnValsMeanX, Response::function_gradients(), Response::function_hessians(), Response::function_values(), Model::hessian_type(), Iterator::iteratedModel, NonD::momentStats, NonDReliability::mppSearchType, Model::multivariate_distribution(), Analyzer::numContinuousVars, Analyzer::numFunctions, NonDLocalReliability::ranVarMeansX, NonDLocalReliability::ranVarStdDevsX, ActiveSet::request_vector(), NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, Iterator::subIteratorFlag, NonDLocalReliability::taylorOrder, and NonDReliability::uSpaceModel.

Referenced by NonDLocalReliability::mean_value(), and NonDLocalReliability::mpp_search().

14.158.2.11 void initialize_class_data ( ) [private]

convenience function for initializing class scope arrays

Initialize class-scope arrays and perform other start-up activities, such as evaluating median limit state responses.

References Response::active_set_derivative_vector(), NonD::finalStatistics, Analyzer::numContinuousVars, Analyzer::numFunctions, NonDReliability::numRelAnalyses, NonDLocalReliability::prevCumASVLev0, NonDLocalReliability::prevFnGradDLev0, NonDLocalReliability::prevFnGradULev0, NonDLocalReliability::prevMPPULev0, Model::probability_transformation(), NonDLocalReliability::ranVarMeansU, NonDLocalReliability::ranVarMeansX, Iterator::subIteratorFlag, NonDReliability::uSpaceModel, and NonDLocalReliability::warmStartFlag.

Referenced by NonDLocalReliability::mpp_search().

14.158.2.12 void initialize_level_data ( ) [private]

convenience function for initializing/warm starting MPP search data for each response function prior to level 0

For a particular response function prior to the first z/p/beta level, initialize/warm-start optimizer initial guess (initialPtU), expansion point (mostProbPointX/U), and associated response data (computedRespLevel, fnGradX/U, and fnHessX/U).

References NonDLocalReliability::assign_mean_data(), NonDLocalReliability::computedRespLevel, Model::inactive_continuous_variables(), NonDLocalReliability::initialPtU, NonDLocalReliability::initialPtUSpec, Iterator::iteratedModel, NonDLocalReliability::mostProbPointU, NonDReliability::mppSearchType, Analyzer::numContinuousVars, NonDReliability::numRelAnalyses, NonDLocalReliability::prevCumASVLev0, NonDLocalReliability::prevFnGradDLev0, NonDLocalReliability::prevFnGradULev0, NonDLocalReliability::prevICVars, NonDLocalReliability::prevMPPULev0, NonD::requestedRespLevels, NonDReliability::respFnCount, Iterator::subIteratorFlag, Model::surrogate_function_indices(), NonDLocalReliability::taylorOrder, NonDLocalReliability::truth_evaluation(), NonDLocalReliability::update_limit_state_surrogate(), NonDReliability::uSpaceModel, and NonDLocalReliability::warmStartFlag.

Referenced by NonDLocalReliability::mpp_search().

14.158.2.13 void initialize_mpp_search_data ( ) [private]

convenience function for initializing/warm starting MPP search data for each z/p/beta level for each response function

For a particular response function at a particular z/p/beta level, warm-start or reset the optimizer initial guess (initialPtU), expansion point (mostProbPointX/U), and associated response data (computedRespLevel, fnGradX/U, and fnHessX/U).

References NonDLocalReliability::assign_mean_data(), NonD::computedGenRelLevels, NonD::computedRelLevels, NonDLocalReliability::fnGradU, Model::hessian_type(), NonDLocalReliability::initialPtU, NonDLocalReliability::initialPtUSpec, NonDLocalReliability::integrationOrder, Iterator::iteratedModel, NonDReliability::levelCount, NonDLocalReliability::mostProbPointU, NonDReliability::mppSearchType, Analyzer::numContinuousVars, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonDReliability::requestedTargetLevel, NonDReliability::respFnCount, NonDLocalReliability::taylorOrder, and NonDLocalReliability::warmStartFlag.

Referenced by NonDLocalReliability::mpp_search().

14.158.2.14 void update_mpp_search_data (const Variables & *vars_star*, const Response & *resp_star*) [private]

convenience function for updating MPP search data for each z/p/beta level for each response function

Includes case-specific logic for updating MPP search data for the AMV/AMV+/TANA/NO_APPROX methods.

References Response::active_set(), Response::active_set_request_vector(), NonDReliability::approxConverged, NonDReliability::approxIters, NonDLocalReliability::computedRelLevel, NonDLocalReliability::computedRespLevel, Model::continuous_variable_ids(), Variables::continuous_variables(), Iterator::convergenceTol, Variables::copy(), Dakota::copy_data(), Model::current_variables(), NonDLocalReliability::curvatureDataAvailable, Dakota::data_pairs, NonD::finalStatistics, NonDLocalReliability::fnGradU, NonDLocalReliability::fnGradX, NonDLocalReliability::fnHessU, NonDLocalReliability::fnHessX, Response::function_values(), NonDLocalReliability::initialPtU, NonDLocalReliability::integrationOrder, Model::interface_id(), Iterator::iteratedModel, NonDLocalReliability::kappaUpdated, NonDReliability::levelCount, Dakota::lookup_by_val(), Iterator::maxIterations, Model::model_rep(), NonDLocalReliability::mostProbPointU, NonDLocalReliability::mostProbPointX, NonDReliability::mppSearchType, Analyzer::numContinuousVars, Analyzer::numFunctions, NonDReliability::pmaMaximizeG, Model::probability_transformation(), ActiveSet::request_vector(), NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonDReliability::requestedTargetLevel, NonDReliability::respFnCount, NonDLocalReliability::signed_norm(), NonDReliability::statCount, NonDLocalReliability::taylorOrder, Model::trans_grad_X_to_U(), Model::trans_hess_X_to_U(), NonDLocalReliability::truth_evaluation(), NonDLocalReliability::update_limit_state_surrogate(), NonDLocalReliability::update_pma_maximize(), NonDReliability::uSpaceModel, NonDLocalReliability::warmStartFlag, and NonDLocalReliability::warningBits.

Referenced by NonDLocalReliability::mpp_search().

14.158.2.15 void update_level_data ( ) [private]

convenience function for updating z/p/beta level data and final statistics following MPP convergence

Updates computedRespLevels/computedProbLevels/computedRelLevels, finalStatistics, warm start, and graphics data.

References Response::active_set_derivative_vector(), Response::active_set_request_vector(), Graphics::add_datapoint(), NonD::cdfFlag, NonDLocalReliability::computedGenRelLevel, NonD::computedGenRelLevels, NonD::computedProbLevels, NonDLocalReliability::computedRelLevel, NonD::computedRelLevels, NonDLocalReliability::computedRespLevel, NonD::computedRespLevels, NonDLocalReliability::dg_ds_eval(), NonDLocalReliability::dp2_dbeta_factor(), NonD::finalStatistics, NonDLocalReliability::fnGradU, NonDLocalReliability::fnGradX, NonDLocalReliability::fnHessU, Response::function_gradient(), OutputManager::graphics(), NonDLocalReliability::integrationOrder, Dakota::length(), NonDReliability::levelCount, NonDLocalReliability::mostProbPointU, NonDLocalReliability::mostProbPointX, Graphics::new_dataset(), Analyzer::numContinuousVars, Analyzer::numFunctions, ParallelLibrary::output_manager(), Iterator::parallelLib, NonDLocalReliability::prevCumASVLev0, NonDLocalReliability::prevFnGradDLev0, NonDLocalReliability::prevFnGradULev0, NonDLocalReliability::prevMPPULev0, NonDLocalReliability::probability(), NonDLocalReliability::reliability(), NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonDReliability::respFnCount, NonD::respLevelTarget, NonD::respLevelTargetReduce, NonDReliability::statCount, Iterator::subIteratorFlag, NonD::totalLevelRequests, and NonDLocalReliability::warmStartFlag.

Referenced by NonDLocalReliability::mpp_search().

14.158.2.16 void dg_ds_eval (const RealVector & *x_vars*, const RealVector & *fn_grad_x*, RealVector & *final_stat_grad*) [private]

convenience function for evaluating dg/ds

Computes dg/ds where s = design variables. Supports potentially overlapping cases of design variable augmentation and insertion.

References Response::active_set_derivative_vector(), Iterator::activeSet, Model::component_parallel_mode(), Model::continuous_variables(), Model::current_response(), ActiveSet::derivative_vector(), Model::evaluate(), NonD::finalStatistics, Response::function_gradient_copy(), Response::function_gradients(), Model::inactive_continuous_variable_ids(), Iterator::iteratedModel, NonDReliability::mppSearchType, Model::nested_acv2_targets(), Model::query_distribution_parameter_derivatives(), ActiveSet::request_value(), ActiveSet::request_values(), NonDReliability::respFnCount, Model::trans_grad_X_to_S(), and NonDReliability::uSpaceModel.

Referenced by NonDLocalReliability::mean_value(), NonDLocalReliability::mpp_search(), and NonDLocalReliability::update_level_data().

14.158.2.17 Real dp2_dbeta_factor (Real *beta*, bool *cdf_flag*) [private]

compute factor for derivative of second-order probability with respect to reliability index (from differentiating BREITUNG or HOHENRACK expressions)

Compute sensitivity of second-order probability w.r.t. beta for use in derivatives of p_2 or beta$*$ w.r.t. auxilliary parameters s (design, epistemic) or derivatives of beta$*$ w.r.t. u in PMA2_constraint_eval().

References Dakota::abort_handler(), NonDLocalReliability::curvatureDataAvailable, NonDLocalReliability::curvatureThresh, NonDLocalReliability::kappaU, Analyzer::numContinuousVars, NonDLocalReliability::probability(), NonDLocalReliability::scale_curvature(), NonDLocalReliability::secondOrderIntType, and NonDLocalReliability::warningBits.

Referenced by NonDLocalReliability::PMA2_constraint_eval(), and NonDLocalReliability::update_level_data().

14.158.2.18 Real probability (Real *beta*, bool *cdf_flag*, const RealVector & *mpp_u*, const RealVector & *fn_grad_u*, const RealSymMatrix & *fn_hess_u*) [private]

Convert provided reliability to probability using either a first-order or second-order integration.

Converts beta into a probability using either first-order (FORM) or second-order (SORM) integration. The SORM calculation first calculates the principal curvatures at the MPP (using the approach in Ch. 8 of Haldar & Mahadevan), and then applies correction formulations from the literature (Breitung, Hohenbichler-Rackwitz, or Hong).

References NonDLocalReliability::curvatureDataAvailable, NonDLocalReliability::curvatureThresh, NonDReliability::importanceSampler, NonDLocalReliability::integrationOrder, NonDReliability::integrationRefinement, Iterator::iterator_rep(), NonDLocalReliability::kappaU, NonDLocalReliability::kappaUpdated, Dakota::length(), NonDReliability::levelCount, Iterator::methodPCIter, NonD::miPLIndex, Analyzer::numContinuousVars, Iterator::outputLevel, NonDLocalReliability::principal_curvatures(), NonDLocalReliability::probability(), NonD::requestedRespLevels, NonDReliability::requestedTargetLevel, NonDReliability::respFnCount, Iterator::run(), NonDLocalReliability::scale_curvature(), NonDLocalReliability::secondOrderIntType, NonDLocalReliability::warningBits, and Dakota::write_precision.

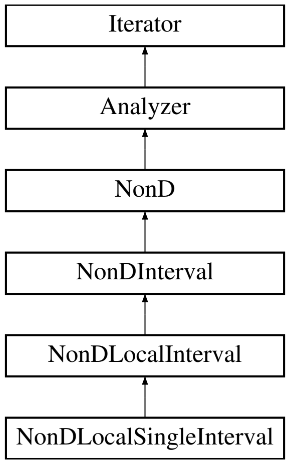
The documentation for this class was generated from the following files:

- NonDLocalReliability.hpp
- NonDLocalReliability.cpp

14.159 NonDLocalSingleInterval Class Reference

Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

Inheritance diagram for NonDLocalSingleInterval:



Public Member Functions

- NonDLocalSingleInterval (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDLocalSingleInterval ()

  destructor

Protected Member Functions

- void initialize ()

  perform any required initialization
- void post_process_cell_results (bool maximize)

  post-process a cell minimization/maximization result

Private Attributes

- size_t statCntr

  counter for finalStatistics

Additional Inherited Members

14.159.1 Detailed Description

Class for using local gradient-based optimization approaches to calculate interval bounds for epistemic uncertainty quantification.

The NonDLocalSingleInterval class supports local gradient-based optimization apporaches to determining interval bounds for epistemic UQ. The interval bounds may be on the entire function in the case of pure interval analysis (e.g. intervals on input = intervals on output), or the intervals may be on statistics of an "inner loop" aleatory analysis such as intervals on means, variances, or percentile levels.

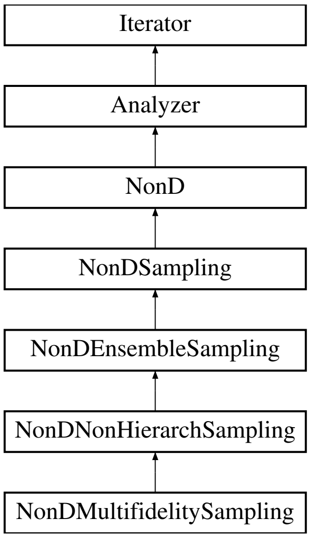
The documentation for this class was generated from the following files:

- NonDLocalSingleInterval.hpp
- NonDLocalSingleInterval.cpp

14.160 NonDMultifidelitySampling Class Reference

Perform Approximate Control Variate Monte Carlo sampling for UQ.

Inheritance diagram for NonDMultifidelitySampling:



Public Member Functions

- NonDMultifidelitySampling (ProblemDescDB &problem_db, Model &model)

  standard constructor
- ∼NonDMultifidelitySampling ()

  destructor

Protected Member Functions

- void core_run ()
- void **print_variance_reduction** (std::ostream &s)
- void multifidelity_mc ()
- void multifidelity_mc_offline_pilot ()
- void multifidelity_mc_pilot_projection ()
- void **mfmc_eval_ratios** (const RealMatrix &var_L, const RealMatrix &rho2_LH, const RealVector &cost, SizetArray &approx_sequence, RealMatrix &eval_ratios, RealVector &hf_targets)
- void **mfmc_numerical_solution** (const RealMatrix &var_L, const RealMatrix &rho2_LH, const RealVector &cost, SizetArray &approx_sequence, RealMatrix &eval_ratios, Real &avg_hf_target)
- void **approx_increments** (IntRealMatrixMap &sum_L_baseline, IntRealVectorMap &sum_H, IntRealMatrixMap &sum_LL, IntRealMatrixMap &sum_LH, const SizetArray &N_H, const SizetArray &approx_sequence, const RealMatrix &eval_ratios, const RealVector &hf_targets)
- bool **mfmc_approx_increment** (const RealMatrix &eval_ratios, const Sizet2DArray &N_L_refined, const RealVector &hf_targets, size_t iter, const SizetArray &approx_sequence, size_t start, size_t end)
- void **update_hf_targets** (const RealMatrix &eval_ratios, const RealVector &cost, RealVector &hf_targets)
- void **update_hf_targets** (const RealMatrix &rho2_LH, const SizetArray &approx_sequence, const RealMatrix &eval_ratios, const RealVector &var_H, const RealVector &estvar_iter0, RealVector &estvar_ratios, RealVector &hf_targets)
- void **update_projected_samples** (const RealVector &hf_targets, const RealMatrix &eval_ratios, SizetArray &N_H_projected, Sizet2DArray &N_L_projected)
- void **mfmc_estimator_variance** (const RealMatrix &rho2_LH, const RealVector &var_H, const SizetArray &N_H, const RealVector &hf_targets, const SizetArray &approx_sequence, const RealMatrix &eval_ratios)

Private Member Functions

- void **initialize_mf_sums** (IntRealMatrixMap &sum_L_baseline, IntRealVectorMap &sum_H, IntRealMatrixMap &sum_LL, IntRealMatrixMap &sum_LH, RealVector &sum_HH)
- void accumulate_mf_sums (IntRealMatrixMap &sum_L_baseline, IntRealVectorMap &sum_H, IntRealMatrixMap &sum_LL, IntRealMatrixMap &sum_LH, RealVector &sum_HH, SizetArray &N_shared)
- void accumulate_mf_sums (RealMatrix &sum_L_baseline, RealVector &sum_H, RealMatrix &sum_LL, RealMatrix &sum_LH, RealVector &sum_HH, SizetArray &N_shared)
- void accumulate_mf_sums (IntRealMatrixMap &sum_L_shared, IntRealMatrixMap &sum_L_refined, Sizet2DArray &num_L_shared, Sizet2DArray &num_L_refined, const SizetArray &approx_sequence, size_t sequence_start, size_t sequence_end)
- void **compute_LH_correlation** (const RealMatrix &sum_L_shared, const RealVector &sum_H, const RealMatrix &sum_LL, const RealMatrix &sum_LH, const RealVector &sum_HH, const SizetArray &N_shared, RealMatrix &var_L, RealVector &var_H, RealMatrix &rho2_LH)
- void **correlation_sq_to_covariance** (const RealMatrix &rho2_LH, const RealMatrix &var_L, const RealVector &var_H, RealMatrix &cov_LH)
- void **matrix_to_diagonal_array** (const RealMatrix &var_L, RealSymMatrixArray &cov_LL)
- void **mf_raw_moments** (IntRealMatrixMap &sum_L_baseline, IntRealMatrixMap &sum_L_shared, IntRealMatrixMap &sum_L_refined, IntRealVectorMap &sum_H, IntRealMatrixMap &sum_LL, IntRealMatrixMap &sum_LH, const Sizet2DArray &num_L_shared, const Sizet2DArray &num_L_refined, const SizetArray &num_H, RealMatrix &H_raw_mom)

Private Attributes

- RealVector estVarRatios

  ratio of MFMC to MC estimator variance for the same HF samples, also known as (1 - R^2)
- unsigned short numericalSolveMode

  controls use of numerical solve option: either a fallback in case of model misordering (default = NUMERICAL_FALLBACK) or override for robustness, e.g., to pilot over-estimation (NUMERICAL_OVERRIDE)

Additional Inherited Members

14.160.1 Detailed Description

Perform Approximate Control Variate Monte Carlo sampling for UQ.

Multifidelity Monte Carlo (MFMC) is a variance-reduction technique that utilitizes lower fidelity simulations that have response QoI that are correlated with the high-fidelity response QoI.

14.160.2 Constructor & Destructor Documentation

14.160.2.1 NonDMultifidelitySampling (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References NonDNonHierarchSampling::mlmfSubMethod.

14.160.3 Member Function Documentation

14.160.3.1 void core_run ( ) [protected], [virtual]

The primary run function manages the general case: a hierarchy of model forms (from the ordered model fidelities within a HierarchSurrModel), each of which may contain multiple discretization levels.

Reimplemented from Iterator.

References NonDMultifidelitySampling::multifidelity_mc(), NonDMultifidelitySampling::multifidelity_mc_offline_-pilot(), NonDMultifidelitySampling::multifidelity_mc_pilot_projection(), NonDNonHierarchSampling::numApprox, NonDSampling::numSamples, NonDEnsembleSampling::pilotMgmtMode, and NonDEnsembleSampling::pilot-Samples.

14.160.3.2 void multifidelity_mc ( ) [protected]

This is the standard MFMC version that integrates the pilot alongside the sample adaptation and iterates to determine numH.

References NonDMultifidelitySampling::accumulate_mf_sums(), NonDNonHierarchSampling::approxSequence, NonDEnsembleSampling::compute_mc_estimator_variance(), NonDEnsembleSampling::estVarIter0, NonD-EnsembleSampling::finalStatsType, NonDNonHierarchSampling::inflate(), Iterator::maxIterations, NonDEnsemble-Sampling::mlmfIter, Analyzer::numFunctions, NonDNonHierarchSampling::numH, NonDNonHierarchSampling-::numHIter0, NonDSampling::numSamples, NonDEnsembleSampling::numSteps, NonDEnsembleSampling-::onlineCost, NonDNonHierarchSampling::recover_online_cost(), NonDNonHierarchSampling::rho2LH, NonD-EnsembleSampling::sequenceCost, and NonDEnsembleSampling::varH.

Referenced by NonDMultifidelitySampling::core_run().

14.160.3.3 void multifidelity_mc_offline_pilot ( ) [protected]

This MFMC version treats the pilot sample as a separate offline process.

References NonDMultifidelitySampling::accumulate_mf_sums(), NonDNonHierarchSampling::approxSequence, NonDEnsembleSampling::finalStatsType, NonDNonHierarchSampling::inflate(), NonDEnsembleSampling::mlmf-Iter, NonDNonHierarchSampling::numApprox, Analyzer::numFunctions, NonDNonHierarchSampling::numH, Non-DSampling::numSamples, NonD::one_sided_delta(), NonDEnsembleSampling::onlineCost, NonDNonHierarch-Sampling::recover_online_cost(), NonDNonHierarchSampling::rho2LH, NonDEnsembleSampling::sequenceCost, and NonDEnsembleSampling::varH.

Referenced by NonDMultifidelitySampling::core_run().

14.160.3.4 void multifidelity_mc_pilot_projection ( ) [protected]

This MFMC version is for algorithm selection; it estimates the variance reduction from pilot-only sampling.

References NonDMultifidelitySampling::accumulate_mf_sums(), NonDNonHierarchSampling::approxSequence, NonDEnsembleSampling::compute_mc_estimator_variance(), NonDEnsembleSampling::estVarIter0, NonD-NonHierarchSampling::inflate(), NonDEnsembleSampling::mlmfIter, NonDNonHierarchSampling::numApprox, Analyzer::numFunctions, NonDNonHierarchSampling::numH, NonDNonHierarchSampling::numHIter0, NonD-Sampling::numSamples, NonDEnsembleSampling::onlineCost, NonDNonHierarchSampling::recover_online_-cost(), NonDNonHierarchSampling::rho2LH, NonDEnsembleSampling::sequenceCost, and NonDEnsemble-Sampling::varH.

Referenced by NonDMultifidelitySampling::core_run().

14.160.3.5 void accumulate_mf_sums (IntRealMatrixMap & *sum_L_baseline,* IntRealVectorMap & *sum_H,* IntRealMatrixMap & *sum_LL,* IntRealMatrixMap & *sum_LH,* RealVector & *sum_HH,* SizetArray & *N_shared*) [private]

Multi-moment map-based, coarse-grained counter version used by MFMC following shared_increment()

References Analyzer::allResponses, Response::function_values(), NonDNonHierarchSampling::numApprox, and Analyzer::numFunctions.

Referenced by NonDMultifidelitySampling::multifidelity_mc(), NonDMultifidelitySampling::multifidelity_mc_offline_-pilot(), and NonDMultifidelitySampling::multifidelity_mc_pilot_projection().

14.160.3.6 void accumulate_mf_sums (RealMatrix & *sum_L_baseline,* RealVector & *sum_H,* RealMatrix & *sum_LL,* RealMatrix & *sum_LH,* RealVector & *sum_HH,* SizetArray & *N_shared*) [private]

Single moment, coarse-grained counter version used by offline-pilot and pilot-projection MFMC following shared_-increment()

References Analyzer::allResponses, Response::function_values(), NonDNonHierarchSampling::numApprox, and Analyzer::numFunctions.

14.160.3.7 void accumulate_mf_sums (IntRealMatrixMap & *sum_L_shared,* IntRealMatrixMap & *sum_L_refined,* Sizet2DArray & *num_L_shared,* Sizet2DArray & *num_L_refined,* const SizetArray & *approx_sequence,* size_t *sequence_start,* size_t *sequence_end*) [private]

```
Multi-moment map-based, fine-grained counter version used by MFMC
following shared_increment()
```

void NonDMultifidelitySampling:: accumulate_mf_sums(IntRealMatrixMap& sum_L_baseline, IntRealVectorMap& sum_H, IntRealMatrixMap& sum_LL, // each L with itself IntRealMatrixMap& sum_LH, // each L with H Real-Vector& sum_HH, Sizet2DArray& num_L_baseline, SizetArray& num_H, Sizet2DArray& num_LH) { uses one set of allResponses with QoI aggregation across all Models, ordered by unorderedModels[i-1], i=1:numApprox –> truthModel

using std::isfinite; Real lf_fn, hf_fn, lf_prod, hf_prod; IntRespMCIter r_it; IntRVMIter h_it; IntRMMIter lb_it, ll_it, lh_it; int lb_ord, h_ord, ll_ord, lh_ord, active_ord, m; size_t qoi, approx, lf_index, hf_index; bool hf_is_finite;

for (r_it=allResponses.begin(); r_it!=allResponses.end(); ++r_it) { const Response& resp = r_it->second; const RealVector& fn_vals = resp.function_values(); const ShortArray& asv = resp.active_set_request_vector();

if (outputLevel >= DEBUG_OUTPUT) { // sample dump for MATLAB checking size_t index = 0; for (approx=0; approx<=numApprox; ++approx) for (qoi=0; qoi<numFunctions; ++qoi, ++index) Cout << fn_vals[index] << ' '; Cout << '

'; }

```
hf_index = numApprox * numFunctions;
for (qoi=0; qoi<numFunctions; ++qoi, ++hf_index) {
  hf_fn = fn_vals[hf_index];
  hf_is_finite = isfinite(hf_fn);
```

High accumulations: if (hf_is_finite) { // neither NaN nor +/-Inf ++num_H[qoi]; High-High: sum_HH[qoi] += hf_fn ∗ hf_fn; // a single vector for ord 1 High: h_it = sum_H.begin(); h_ord = (h_it == sum_H.end()) ? 0 : h_it->first; hf_prod = hf_fn; active_ord = 1; while (h_ord) { if (h_ord == active_ord) { // support general key sequence h_it->second[qoi] += hf_prod; ++h_it; h_ord = (h_it == sum_H.end()) ? 0 : h_it->first; } hf_prod ∗= hf_fn; ++active_ord; } }

for (approx=0; approx<numApprox; ++approx) { lf_index = approx ∗ numFunctions + qoi; lf_fn = fn_vals[lf_index];

Low accumulations: if (isfinite(lf_fn)) { ++num_L_baseline[approx][qoi]; if (hf_is_finite) ++num_LH[approx][qoi];

lb_it = sum_L_baseline.begin(); ll_it = sum_LL.begin(); lh_it = sum_LH.begin(); lb_ord = (lb_it == sum_L_baseline.-end()) ? 0 : lb_it->first; ll_ord = (ll_it == sum_LL.end()) ? 0 : ll_it->first; lh_ord = (lh_it == sum_LH.end()) ? 0 : lh_it->first; lf_prod = lf_fn; hf_prod = hf_fn; active_ord = 1; while (lb_ord || ll_ord || lh_ord) {

Low baseline if (lb_ord == active_ord) { // support general key sequence lb_it->second(qoi,approx) += lf_prod; ++lb_it; lb_ord = (lb_it == sum_L_baseline.end()) ? 0 : lb_it->first; } Low-Low if (ll_ord == active_ord) { // support general key sequence ll_it->second(qoi,approx) += lf_prod ∗ lf_prod; ++ll_it; ll_ord = (ll_it == sum_LL.end()) ? 0 : ll_it->first; } Low-High if (lh_ord == active_ord) { if (hf_is_finite) lh_it->second(qoi,approx) += lf_prod ∗ hf_prod; ++lh_it; lh_ord = (lh_it == sum_LH.end()) ? 0 : lh_it->first; }

lf_prod ∗= lf_fn; ++active_ord; if (hf_is_finite) hf_prod ∗= hf_fn; } } } } } } Single moment, fine-grained counter version used by offline-pilot and pilot-projection MFMC following shared_increment() void NonDMultifidelitySampling:: accumulate_mf_sums(RealMatrix& sum_L_baseline, RealVector& sum_H, RealMatrix& sum_LL, RealMatrix& sum-_LH, RealVector& sum_HH, Sizet2DArray& num_L_baseline, SizetArray& num_H, Sizet2DArray& num_LH) { uses one set of allResponses with QoI aggregation across all Models, ordered by unorderedModels[i-1], i=1:numApprox –> truthModel using std::isfinite; Real lf_fn, hf_fn; size_t qoi, approx, lf_index, hf_index; IntRespMCIter r_it; bool hf_is_finite;

for (r_it=allResponses.begin(); r_it!=allResponses.end(); ++r_it) { const Response& resp = r_it->second; const RealVector& fn_vals = resp.function_values(); const ShortArray& asv = resp.active_set_request_vector();

if (outputLevel >= DEBUG_OUTPUT) { // sample dump for MATLAB checking size_t index = 0; for (approx=0; approx<=numApprox; ++approx) for (qoi=0; qoi<numFunctions; ++qoi, ++index) Cout << fn_vals[index] << ' '; Cout << '

'; }

```
hf_index = numApprox * numFunctions;
for (qoi=0; qoi<numFunctions; ++qoi, ++hf_index) {
  hf_fn = fn_vals[hf_index];
  hf_is_finite = isfinite(hf_fn);
```

High accumulations: if (hf_is_finite) { // neither NaN nor +/-Inf ++num_H[qoi]; sum_H[qoi] += hf_fn; // High sum_H-H[qoi] += hf_fn $*$ hf_fn; // High-High }

for (approx=0; approx<numApprox; ++approx) { lf_index = approx $*$ numFunctions + qoi; lf_fn = fn_vals[lf_index];

Low accumulations: if (isfinite(lf_fn)) { ++num_L_baseline[approx][qoi]; sum_L_baseline(qoi,approx) += lf_fn; // Low sum_LL(qoi,approx) += lf_fn $*$ lf_fn; // Low-Low if (hf_is_finite) { ++num_LH[approx][qoi]; sum_LH(qoi,approx) += lf_fn $*$ hf_fn;// Low-High } } } } } }This version used by MFMC following approx_increment()

References Analyzer::allResponses, Response::function_values(), and Analyzer::numFunctions.

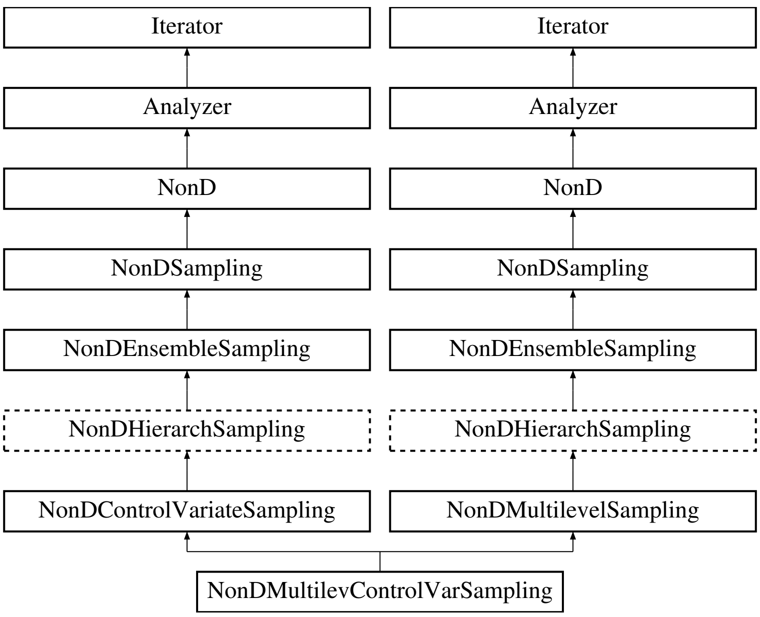
The documentation for this class was generated from the following files:

- NonDMultifidelitySampling.hpp
- NonDMultifidelitySampling.cpp

14.161 NonDMultilevControlVarSampling Class Reference

Performs multilevel-multifidelity Monte Carlo sampling for uncertainty quantification.

Inheritance diagram for NonDMultilevControlVarSampling:



Public Member Functions

- NonDMultilevControlVarSampling (ProblemDescDB &problem_db, Model &model)

standard constructor
- ∼NonDMultilevControlVarSampling ()

  destructor

Protected Member Functions

- void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()
- void **print_variance_reduction** (std::ostream &s)

Private Member Functions

- void multilevel_control_variate_mc_Qcorr ()

  Perform multilevel Monte Carlo across levels in combination with control variate Monte Carlo across model forms at each level; CV computes correlations for Q (LH correlations for QoI)
- void multilevel_control_variate_mc_offline_pilot ()

  Qcorr approach using a pilot sample treated as separate offline cost.
- void multilevel_control_variate_mc_pilot_projection ()

  Qcorr approach projecting estimator performance from a pilot sample.
- void evaluate_pilot (RealVector &hf_cost, RealVector &lf_cost, RealVectorArray &eval_ratios, RealMatrix &Lambda, RealMatrix &var_YH, Sizet2DArray &N_shared, RealVector &hf_targets, bool accumulate_cost, bool pilot_estvar)

  helper for shared code among offline-pilot and pilot-projection modes
- void compute_mlmf_equivalent_cost (const SizetArray &raw_N_hf, const RealVector &hf_cost, const SizetArray &raw_N_lf, const RealVector &lf_cost)

  compute the equivalent number of HF evaluations (includes any sim faults)
- void increment_mlmf_equivalent_cost (size_t new_N_hf, Real hf_lev_cost, size_t new_N_lf, Real lf_lev_cost, Real hf_ref_cost)

  increment the equivalent number of HF evaluations
- void compute_mlmf_estimator_variance (const RealMatrix &var_Y, const Sizet2DArray &num_Y, const RealMatrix &Lambda, RealVector &mlmf_est_var)

  compute the variance of the MLMF estimator
- void compute_eval_ratios (RealMatrix &sum_L_shared, RealMatrix &sum_H, RealMatrix &sum_LL, RealMatrix &sum_LH, RealMatrix &sum_HH, Real cost_ratio, size_t lev, const SizetArray &N_shared, RealMatrix &var_H, RealMatrix &rho2_LH, RealVector &eval_ratios)

  compute the LF/HF evaluation ratio, averaged over the QoI
- void compute_eval_ratios (RealMatrix &sum_Ll, RealMatrix &sum_Llm1, RealMatrix &sum_Hl, RealMatrix &sum_Hlm1, RealMatrix &sum_Ll_Ll, RealMatrix &sum_Ll_Llm1, RealMatrix &sum_Llm1_Llm1, RealMatrix &sum_Hl_Ll, RealMatrix &sum_Hl_Llm1, RealMatrix &sum_Hlm1_Ll, RealMatrix &sum_Hlm1_Llm1, RealMatrix &sum_Hl_Hl, RealMatrix &sum_Hl_Hlm1, RealMatrix &sum_Hlm1_Hlm1, Real cost_ratio, size_t lev, const SizetArray &N_shared, RealMatrix &var_YHl, RealMatrix &rho_dot2_LH, RealVector &eval_ratios)

  compute the LF/HF evaluation ratio, averaged over the QoI
- void cv_raw_moments (IntRealMatrixMap &sum_L_shared, IntRealMatrixMap &sum_H, IntRealMatrixMap &sum_LL, IntRealMatrixMap &sum_LH, const SizetArray &N_shared, IntRealMatrixMap &sum_L_refined, const SizetArray &N_refined, size_t lev, RealMatrix &H_raw_mom)

  apply control variate parameters for MLMF MC to estimate raw moment contributions
- void cv_raw_moments (IntRealMatrixMap &sum_Ll, IntRealMatrixMap &sum_Llm1, IntRealMatrixMap &sum_Hl, IntRealMatrixMap &sum_Hlm1, IntRealMatrixMap &sum_Ll_Ll, IntRealMatrixMap &sum_Ll_Llm1, IntRealMatrixMap &sum_Llm1_Llm1, IntRealMatrixMap &sum_Hl_Ll, IntRealMatrixMap &sum_Hl_Llm1, IntRealMatrixMap &sum_Hlm1_Ll, IntRealMatrixMap &sum_Hlm1_Llm1, IntRealMatrixMap &sum_Hl_Hl, IntRealMatrixMap &sum_Hl_Hlm1, IntRealMatrixMap &sum_Hlm1_Hlm1, const SizetArray &N_shared, IntRealMatrixMap &sum_Ll_refined, IntRealMatrixMap &sum_Llm1_refined, const SizetArray &N_refined, size_t lev, RealMatrix &H_raw_mom)

apply control variate parameters for MLMF MC to estimate raw moment contributions

- void compute_mlmf_control (Real sum_Ll, Real sum_Llm1, Real sum_Hl, Real sum_Hlm1, Real sum_Ll_Ll, Real sum_Ll_Llm1, Real sum_Llm1_Llm1, Real sum_Hl_Ll, Real sum_Hl_Llm1, Real sum_Hlm1_Ll, Real sum_Hlm1_Llm1, Real sum_Hl_Hl, Real sum_Hl_Hlm1, Real sum_Hlm1_Hlm1, size_t N_shared, Real &var_YHl, Real &rho_dot2_LH, Real &beta_dot, Real &gamma)

  compute scalar control variate parameters
- void compute_mlmf_control (const RealMatrix &sum_Ll, const RealMatrix &sum_Llm1, const RealMatrix &sum_Hl, const RealMatrix &sum_Hlm1, const RealMatrix &sum_Ll_Ll, const RealMatrix &sum_Ll_Llm1, const RealMatrix &sum_Llm1_Llm1, const RealMatrix &sum_Hl_Ll, const RealMatrix &sum_Hl_Llm1, const RealMatrix &sum_Hlm1_Ll, const RealMatrix &sum_Hlm1_Llm1, const RealMatrix &sum_Hl_Hl, const RealMatrix &sum_Hl_Hlm1, const RealMatrix &sum_Hlm1_Hlm1, const SizetArray &N_shared, size_t lev, RealVector &beta_dot, RealVector &gamma)

  compute matrix control variate parameters
- void apply_mlmf_control (Real sum_Hl, Real sum_Hlm1, Real sum_Ll, Real sum_Llm1, size_t N_shared, Real sum_Ll_refined, Real sum_Llm1_refined, size_t N_refined, Real beta_dot, Real gamma, Real &H_raw_mom)

  apply scalar control variate parameter (beta) to approximate HF moment
- void apply_mlmf_control (const RealMatrix &sum_Hl, const RealMatrix &sum_Hlm1, const RealMatrix &sum_Ll, const RealMatrix &sum_Llm1, const SizetArray &N_shared, const RealMatrix &sum_Ll_refined, const RealMatrix &sum_Llm1_refined, const SizetArray &N_refined, size_t lev, const RealVector &beta_dot, const RealVector &gamma, RealVector &H_raw_mom)

  apply matrix control variate parameter (beta) to approximate HF moment
- void update_projected_samples (const RealVector &hf_targets, const RealVectorArray &eval_ratios, Sizet2DArray &N_hf, const RealVector &hf_cost, Sizet2DArray &N_lf, const RealVector &lf_cost)

  for pilot projection mode, advance sample counts and accumulated cost
- void initialize_mlmf_sums (IntRealMatrixMap &sum_L_shared, IntRealMatrixMap &sum_L_refined, IntRealMatrixMap &sum_H, IntRealMatrixMap &sum_LL, IntRealMatrixMap &sum_LH, IntRealMatrixMap &sum_HH, size_t num_ml_lev, size_t num_cv_lev)

  initialize the MLMF accumulators for computing means, variances, and covariances across fidelity levels
- void initialize_mlmf_sums (IntRealMatrixMap &sum_Ll, IntRealMatrixMap &sum_Llm1, IntRealMatrixMap &sum_Ll_refined, IntRealMatrixMap &sum_Llm1_refined, IntRealMatrixMap &sum_Hl, IntRealMatrixMap &sum_Hlm1, IntRealMatrixMap &sum_Ll_Ll, IntRealMatrixMap &sum_Ll_Llm1, IntRealMatrixMap &sum_Llm1_Llm1, IntRealMatrixMap &sum_Hl_Ll, IntRealMatrixMap &sum_Hl_Llm1, IntRealMatrixMap &sum_Hlm1_Ll, IntRealMatrixMap &sum_Hlm1_Llm1, IntRealMatrixMap &sum_Hl_Hl, IntRealMatrixMap &sum_Hl_Hlm1, IntRealMatrixMap &sum_Hlm1_Hlm1, size_t num_ml_lev, size_t num_cv_lev)

  initialize the MLMF accumulators for computing means, variances, and covariances across fidelity levels
- void accumulate_mlmf_Qsums (IntRealMatrixMap &sum_Ql, IntRealMatrixMap &sum_Qlm1, size_t lev, SizetArray &num_Q)

  update running QoI sums for one model at two levels (sum_Ql, sum_Qlm1) using set of model evaluations within allResponses
- void accumulate_mlmf_Ysums (IntRealMatrixMap &sum_Y, size_t lev, SizetArray &num_Y)

  update running discrepancy sums for one model (sum_Y) using set of model evaluations within allResponses
- void accumulate_mlmf_Qsums (const IntResponseMap &lf_resp_map, const IntResponseMap &hf_resp_map, IntRealMatrixMap &sum_L_shared, IntRealMatrixMap &sum_L_refined, IntRealMatrixMap &sum_H, IntRealMatrixMap &sum_LL, IntRealMatrixMap &sum_LH, IntRealMatrixMap &sum_HH, size_t lev, SizetArray &num_L, SizetArray &num_H)

  update running QoI sums for two models (sum_L, sum_H, sum_LL, sum_LH, and sum_HH) from set of low/high fidelity model evaluations within {lf,hf}_resp_map; used for level 0 from other accumulators
- void accumulate_mlmf_Qsums (const IntResponseMap &lf_resp_map, const IntResponseMap &hf_resp_map, RealMatrix &sum_L_shared, RealMatrix &sum_L_refined, RealMatrix &sum_H, RealMatrix &sum_LL, RealMatrix &sum_LH, RealMatrix &sum_HH, size_t lev, SizetArray &N_shared)

  update running QoI sums for two models (sum_L, sum_H, sum_LL, sum_LH, and sum_HH) from set of low/high fidelity model evaluations within {lf,hf}_resp_map; used for level 0 from other accumulators

- void accumulate_mlmf_Ysums (const IntResponseMap &lf_resp_map, const IntResponseMap &hf_resp_-map, IntRealMatrixMap &sum_L_shared, IntRealMatrixMap &sum_L_refined, IntRealMatrixMap &sum_H, IntRealMatrixMap &sum_LL, IntRealMatrixMap &sum_LH, IntRealMatrixMap &sum_HH, size_t lev, Sizet-Array &num_L, SizetArray &num_H)

  update running two-level discrepancy sums for two models (sum_L, sum_H, sum_LL, sum_LH, and sum_HH) from set of low/high fidelity model evaluations within {lf,hf}resp_map
- void accumulate_mlmf_Qsums (const IntResponseMap &lf_resp_map, const IntResponseMap &hf_resp_-map, IntRealMatrixMap &sum_Ll, IntRealMatrixMap &sum_Llm1, IntRealMatrixMap &sum_Ll_refined, Int-RealMatrixMap &sum_Llm1_refined, IntRealMatrixMap &sum_Hl, IntRealMatrixMap &sum_Hlm1, IntReal-MatrixMap &sum_Ll_Ll, IntRealMatrixMap &sum_Ll_Llm1, IntRealMatrixMap &sum_Llm1_Llm1, IntReal-MatrixMap &sum_Hl_Ll, IntRealMatrixMap &sum_Hl_Llm1, IntRealMatrixMap &sum_Hlm1_Ll, IntRealMatrix-Map &sum_Hlm1_Llm1, IntRealMatrixMap &sum_Hl_Hl, IntRealMatrixMap &sum_Hl_Hlm1, IntRealMatrix-Map &sum_Hlm1_Hlm1, size_t lev, SizetArray &num_L, SizetArray &num_H)

  update running QoI sums for two models and two levels from set of low/high fidelity model evaluations within {lf,hf}_-resp_map
- void accumulate_mlmf_Qsums (const IntResponseMap &lf_resp_map, const IntResponseMap &hf_resp_-map, RealMatrix &sum_Ll, RealMatrix &sum_Llm1, RealMatrix &sum_Ll_refined, RealMatrix &sum_Llm1_-refined, RealMatrix &sum_Hl, RealMatrix &sum_Hlm1, RealMatrix &sum_Ll_Ll, RealMatrix &sum_Ll_Llm1, RealMatrix &sum_Llm1_Llm1, RealMatrix &sum_Hl_Ll, RealMatrix &sum_Hl_Llm1, RealMatrix &sum_Hlm1-_Ll, RealMatrix &sum_Hlm1_Llm1, RealMatrix &sum_Hl_Hl, RealMatrix &sum_Hl_Hlm1, RealMatrix &sum-_Hlm1_Hlm1, size_t lev, SizetArray &N_shared)

  update running QoI sums for two models and two levels from set of low/high fidelity model evaluations within {lf,hf}_-resp_map

Private Attributes

- short delegateMethod

  core_run() can delegate execution to either ML or CV if hierarchy does not support MLCV; in this case output must also be delegated

Additional Inherited Members

14.161.1 Detailed Description

Performs multilevel-multifidelity Monte Carlo sampling for uncertainty quantification.

Multilevel-multifidelity Monte Carlo (MLMFMC) combines variance decay across model resolutions with variance reduction from a control variate across model fidelities.

14.161.2 Constructor & Destructor Documentation

14.161.2.1 NonDMultilevControlVarSampling (ProblemDescDB & *problem_db*, Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Iterator::iteratedModel, and Model::multilevel_multifidelity().

14.161.3 Member Function Documentation

14.161.3.1 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from NonDEnsembleSampling.

References NonDEnsembleSampling::NLev, Analyzer::numFunctions, and NonDEnsembleSampling::pre_run().

14.161.3.2 void core_run ( ) [protected], [virtual]

The primary run function manages the general case: a hierarchy of model forms (from the ordered model fidelities within a HierarchSurrModel), each of which may contain multiple discretization levels.

Reimplemented from NonDControlVariateSampling.

References Model::active_model_key(), NonDControlVariateSampling::core_run(), NonDMultilevelSampling::core_run(), NonDMultilevControlVarSampling::delegateMethod, Iterator::iteratedModel, NonDMultilevControlVarSampling::multilevel_control_variate_mc_offline_pilot(), NonDMultilevControlVarSampling::multilevel_control_variate_mc_pilot_projection(), NonDMultilevControlVarSampling::multilevel_control_variate_mc_Qcorr(), NonDEnsembleSampling::NLev, NonDEnsembleSampling::pilotMgmtMode, NonDEnsembleSampling::sequenceType, Model::subordinate_models(), and Dakota::SZ_MAX.

14.161.3.3 void multilevel_control_variate_mc_Qcorr ( ) [private]

Perform multilevel Monte Carlo across levels in combination with control variate Monte Carlo across model forms at each level; CV computes correlations for Q (LH correlations for QoI)

```
This function performs "geometrical" MLMC across discretization
levels for the high fidelity model form where CVMC si employed
across two model forms to exploit correlation in the discrepancies
at each level (Y_l).
```

void NonDMultilevControlVarSampling::multilevel_control_variate_mc_Ycorr() { Model& truth_model = iteratedModel.truth_model(); Model& surr_model = iteratedModel.surrogate_model(); size_t qoi, lev, num_mf = NLev.size(), num_hf_lev = truth_model.solution_levels(), num_cv_lev = std::min(num_hf_lev, surr_model.solution_levels()); bool budget_constrained = (maxFunctionEvals != SZ_MAX);

retrieve cost estimates across solution levels for HF model RealVector hf_targets(num_hf_lev), agg_var_hf(num_hf_lev), hf_cost = truth_model.solution_level_costs(), lf_cost = surr_model.solution_level_costs(); Real eps_sq_div_2, sum_sqrt_var_cost, agg_estvar_iter0 = 0., budget, r_lq, lf_lev_cost, hf_lev_cost, hf_ref_cost = hf_cost[num_hf_lev-1]; if (budget_constrained) budget = (Real)maxFunctionEvals ∗ hf_ref_cost; RealVectorArray eval_ratios(num_cv_lev); For moment estimation, we accumulate telescoping sums for Q^i using discrepancies Yi = Q^i_{lev} - Q^i_{lev-1} (Y_diff_Qpow[i] for i=1:4). For computing N_l from estimator variance, we accumulate square of Y1 estimator (YY[1] = (Y^i)^2 for i=1). IntRealMatrixMap sum_L_refined, sum_L_shared, sum_H, sum_LL, sum_LH, sum_HH; initialize_mlmf_sums(sum_L_shared, sum_L_refined, sum_H, sum_LL, sum_LH, sum_HH, num_hf_lev, num_cv_lev); RealMatrix var_YH(numFunctions, num_hf_lev, false), rho2_LH(numFunctions, num_cv_lev, false), Lambda(numFunctions, num_cv_lev, false); RealVector avg_rho2_LH(num_cv_lev, false), avg_lambda(num_cv_lev, false);

Initialize for pilot sample unsigned short group, lf_form = 0, hf_form = num_mf - 1;// 2 models @ extremes Sizet2DArray& N_lf = NLev[lf_form]; Sizet2DArray& N_hf = NLev[hf_form]; Sizet2DArray delta_N_l; load_pilot_sample(pilotSamples, NLev, delta_N_l); SizetArray& delta_N_lf = delta_N_l[lf_form]; SizetArray& delta_N_hf = delta_N_l[hf_form];

now converge on sample counts per level (N_hf) while (Pecos::l1_norm(delta_N_hf) && mlmfIter <= maxIterations) {

sum_sqrt_var_cost = 0.; for (lev=0, group=0; lev<num_hf_lev; ++lev, ++group) {

configure_indices(group, hf_form, lev, sequenceType); hf_lev_cost = level_cost(hf_cost, lev);

set the number of current samples from the defined increment numSamples = delta_N_hf[lev];

aggregate variances across QoI for estimating N_hf (justification: for independent QoI, sum of QoI variances = variance of QoI sum) Real& agg_var_hf_l = agg_var_hf[lev];//carried over from prev iter if!samp if (numSamples) {

assign sequence, get samples, export, evaluate evaluate_ml_sample_increment(lev);

control variate betwen LF and HF for this discretization level: if unequal number of levels, loop over all HF levels for MLMC and apply CVMC when LF levels are available. LF levels are assigned as control variates to the leading set of HF levels, since these will tend to have larger variance. if (lev < num_cv_lev) {

store allResponses used for sum_H (and sum_HH) IntResponseMap hf_resp = allResponses; // shallow copy activate LF response (lev 0) or LF response discrepancy (lev > 0) within the hierarchical surrogate model. Level indices & surrogate response mode are same as HF above, only the model form changes. However, we must pass the unchanged level index to update the corresponding variable values for the new model form. configure_indices(group, lf_form, lev, sequenceType); lf_lev_cost = level_cost(lf_cost, lev); compute allResp w/ LF model form reusing allVars from MLMC step evaluate_parameter_sets(iteratedModel, true, false); process previous and new set of allResponses for CV sums accumulate_mlmf_Ysums(allResponses, hf_resp, sum_L_shared, sum_L_refined, sum_H, sum_LL, sum_LH, sum_HH, lev, N_lf[lev], N_hf[lev]); if (outputLevel == DEBUG_OUTPUT) Cout << "Accumulated sums (L_shared[1,2], L_refined[1,2], LH[1,2])" << ":\n" << sum_L_shared[1] << sum_L_shared[2] << sum_L_refined[1]<< sum_L_refined[2]<< sum_LH[1]<< sum_LH[2]; increment_mlmf_equivalent_cost(numSamples, hf_lev_cost, numSamples, lf_lev_cost, hf_ref_cost);

compute the average evaluation ratio and Lambda factor RealVector& eval_ratios_l = eval_ratios[lev]; compute_eval_ratios(sum_L_shared[1], sum_H[1], sum_LL[1], sum_LH[1], sum_HH[1], hf_lev_cost/lf_lev_cost, lev, N_hf[lev], var_YH, rho2_LH, eval_ratios_l);

retain Lambda per QoI and level, but apply QoI-average where needed for (qoi=0; qoi<numFunctions; ++qoi) { r_lq = eval_ratios_l[qoi]; Lambda(qoi,lev) = 1. - rho2_LH(qoi,lev) * (r_lq - 1.) / r_lq; } avg_lambda[lev] = average(Lambda[lev], numFunctions); avg_rho2_LH[lev] = average(rho2_LH[lev], numFunctions); } else { // no LF model for this level; accumulate only multilevel sums RealMatrix& sum_HH1 = sum_HH[1]; accumulate H sums for lev = 0, Y sums for lev > 0 accumulate_ml_Ysums(sum_H, sum_HH1, lev, N_hf[lev]); if (outputLevel == DEBUG_OUTPUT) Cout << "Accumulated sums (H[1], H[2], HH):\n" << sum_H[1] << sum_H[2] << sum_HH1; increment_ml_equivalent_cost(numSamples, hf_lev_cost, hf_ref_cost); compute Y variances for this level and aggregate across QoI: variance_Ysum(sum_H[1][lev], sum_HH1[lev], N_hf[lev], var_YH[lev]); } agg_var_hf_l = sum(var_YH[lev], numFunctions); }

accumulate sum of sqrt's of estimator var * cost used in N_target if (lev < num_cv_lev) { Real om_rho2 = 1. - avg_rho2_LH[lev]; sum_sqrt_var_cost += (budget_constrained) ? std::sqrt(agg_var_hf_l / hf_lev_cost * om_rho2) * (hf_lev_cost + (1. + average(eval_ratios[lev])) * lf_lev_cost) : std::sqrt(agg_var_hf_l * hf_lev_cost / om_rho2) * avg_lambda[lev]; } else sum_sqrt_var_cost += std::sqrt(agg_var_hf_l * hf_lev_cost);

MSE reference is MLMF MC applied to {HF,LF} pilot sample aggregated across qoi. Note: if the pilot sample for LF is not shaped, then r=1 will result in no additional variance reduction beyond MLMC. if (mlmfIter == 0 && !budget_constrained) agg_estvar_iter0 += aggregate_mse_Yvar(var_YH[lev], N_hf[lev]); } compute epsilon target based on relative tolerance: total MSE = eps^2 which is equally apportioned (eps^2 / 2) among discretization MSE and estimator variance (var_Y_l / N_l). Since we do not know the discretization error, we compute an initial estimator variance and then seek to reduce it by a relative_factor <= 1. if (mlmfIter == 0) { MLMC estimator variance for final estvar reporting is not aggregated (reduction from control variate is applied subsequently) compute_ml_estimator_variance(var_YH, N_hf, estVarIter0);//numHIter0=numH; compute eps^2 / 2 = aggregated estvar0 * rel tol if (!budget_constrained) { eps_sq_div_2 = agg_estvar_iter0 * convergenceTol; if (outputLevel == DEBUG_OUTPUT) Cout << "Epsilon squared target = " << eps_sq_div_2 << std::endl; } }

update sample targets based on variance estimates Note: sum_sqrt_var_cost is defined differently for the two cases Real fact = (budget_constrained) ? budget / sum_sqrt_var_cost : // budget constraint sum_sqrt_var_cost / eps_sq_div_2; // error balance constraint for (lev=0; lev<num_hf_lev; ++lev) { hf_lev_cost = (lev) ? hf_cost[lev] + hf_cost[lev-1] : hf_cost[lev]; hf_targets[lev] = (lev < num_cv_lev) ? fact * std::sqrt(agg_var_hf[lev] / hf_lev_cost * (1. - avg_rho2_LH[lev])) : fact * std::sqrt(agg_var_hf[lev] / hf_lev_cost); delta_N_hf[lev] = one_sided_delta(average(N_hf[lev]), hf_targets[lev]); }

++mlmfIter; Cout << "\nMLMF MC iteration " << mlmfIter << " sample increments:\n" << delta_N_hf << std::endl; }

All CV lf_increment() calls now follow convergence of ML iteration: for (lev=0, group=0; lev<num_cv_lev; ++lev, ++group) { configure_indices(group, lf_form, lev, sequenceType); execute additional LF sample increment if (lf_-

increment(eval_ratios[lev], N_lf[lev], hf_targets[lev], mlmfIter, lev)) { accumulate_mlmf_Ysums(sum_L_refined, lev, N_lf[lev]); increment_ml_equivalent_cost(numSamples, level_cost(lf_cost, lev), hf_ref_cost); if (outputLevel == DEBUG_OUTPUT) Cout << "Accumulated sums (L_refined[1,2]):\n" << sum_L_refined[1] << sum_L_refined[2]; } }

Roll up raw moments from MLCVMC and MLMC levels RealMatrix Y_mom(numFunctions, 4), Y_cvmc_mom(numFunctions, 4, false); for (lev=0; lev<num_cv_lev; ++lev) { cv_raw_moments(sum_L_shared, sum_H, sum_LL, sum_LH, N_hf[lev], sum_L_refined, N_lf[lev], //rho2_LH, lev, Y_cvmc_mom); Y_mom += Y_cvmc_mom; } if (num_hf_lev > num_cv_lev) ml_raw_moments(sum_H[1], sum_H[2], sum_H[3], sum_H[4], N_hf, num_cv_lev, num_hf_lev, Y_mom); convert_moments(Y_mom, momentStats); // raw to final (central or std) recover_variance(momentStats, varH);

compute_mlmf_estimator_variance(var_YH, N_hf, Lambda, estVar); avgEstVar = average(estVar); }This function performs "geometrical" MLMC across discretization levels for the high fidelity model form where CVMC is employed across two model forms. It generalizes the Y_l correlation case to separately target correlations for each QoI level embedded within the level discrepancies.

References NonDMultilevelSampling::accumulate_ml_Ysums(), NonDMultilevControlVarSampling::accumulate_mlmf_Qsums(), NonDHierarchSampling::accumulate_paired_online_cost(), NonDMultilevelSampling::aggregate_mse_Yvar(), Analyzer::allResponses, NonDEnsembleSampling::average(), NonDHierarchSampling::average_online_cost(), NonDEnsembleSampling::avgEstVar, NonDMultilevControlVarSampling::compute_eval_ratios(), NonDMultilevelSampling::compute_ml_estimator_variance(), NonDMultilevControlVarSampling::compute_mlmf_estimator_variance(), NonDMultilevelSampling::configure_indices(), Iterator::convergenceTol, NonDEnsembleSampling::convert_moments(), NonDMultilevControlVarSampling::cv_raw_moments(), NonDMultilevelSampling::estVar, NonDEnsembleSampling::estVarIter0, NonDMultilevelSampling::evaluate_ml_sample_increment(), Analyzer::evaluate_parameter_sets(), NonDEnsembleSampling::finalStatsType, NonDMultilevelSampling::increment_ml_equivalent_cost(), NonDMultilevControlVarSampling::increment_mlmf_equivalent_cost(), NonDMultilevControlVarSampling::initialize_mlmf_sums(), Iterator::iteratedModel, NonDMultilevelSampling::level_cost(), NonDControlVariateSampling::lf_increment(), NonD::load_pilot_sample(), Iterator::maxFunctionEvals, Iterator::maxIterations, NonDMultilevelSampling::ml_raw_moments(), NonDEnsembleSampling::mlmfIter, NonD::momentStats, NonDEnsembleSampling::NLev, Analyzer::numFunctions, NonDSampling::numSamples, NonD::one_sided_delta(), Iterator::outputLevel, NonDEnsembleSampling::pilotSamples, NonD::query_cost(), NonDMultilevelSampling::recover_variance(), NonDEnsembleSampling::sequenceType, Model::solution_levels(), NonDEnsembleSampling::sum(), Model::surrogate_model(), Dakota::SZ_MAX, Model::truth_model(), NonDMultilevControlVarSampling::update_projected_samples(), NonDEnsembleSampling::varH, and NonDMultilevelSampling::variance_Ysum().

Referenced by NonDMultilevControlVarSampling::core_run().

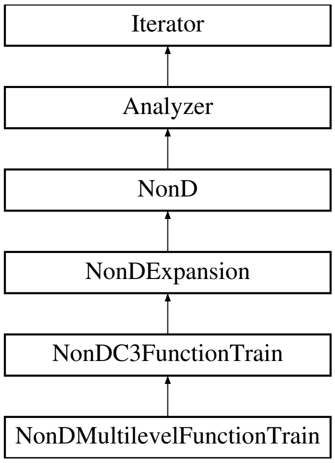
The documentation for this class was generated from the following files:

- NonDMultilevControlVarSampling.hpp
- NonDMultilevControlVarSampling.cpp

14.162 NonDMultilevelFunctionTrain Class Reference

Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.

Inheritance diagram for NonDMultilevelFunctionTrain:



Public Member Functions

- NonDMultilevelFunctionTrain (ProblemDescDB &problem_db, Model &model)

    standard constructor
- ∼NonDMultilevelFunctionTrain ()

    destructor

Protected Member Functions

- void initialize_u_space_model ()

    initialize uSpaceModel polynomial approximations with PCE/SC data
- void core_run ()

    perform a forward uncertainty propagation using PCE/SC methods
- void assign_specification_sequence ()

    assign the current values from the input specification sequence
- void increment_specification_sequence ()

    increment the input specification sequence and assign values
- size_t collocation_points () const

    return specification for number of collocation points (may be part of a sequence specification)
- int random_seed () const

    return specification for random seed (may be part of a sequence specification)
- int first_seed () const

    return first seed in sequence specification (defaults to random_seed())
- void initialize_ml_regression (size_t num_lev, bool &import_pilot)

    initializations for multilevel_regression()
- void infer_pilot_sample (size_t num_steps, SizetArray &delta_N_l)
- void increment_sample_sequence (size_t new_samp, size_t total_samp, size_t step)

    increment sequence in numSamplesOnModel for multilevel_regression()
- void compute_sample_increment (const RealVector &regress_metrics, const SizetArray &N_l, SizetArray &delta_N_l)

    compute delta_N_l for {RIP,RANK}_SAMPLING cases
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

    print the final statistics
- void assign_allocation_control ()

    assign defaults related to allocation control (currently for ML regression approaches)

Private Member Functions

- size_t **start_rank** (size_t index) const
- size_t **start_rank** () const
- unsigned short **start_order** (size_t index) const
- unsigned short **start_order** () const
- void **push_c3_active** (const UShortArray &orders)
- void **push_c3_active** ()
- size_t regression_size (size_t index)

    return the regression size used for different refinement options; the index identifies the point in the specification sequence

Private Attributes

- SizetArray startRankSeqSpec

    user specification for start_rank_sequence
- UShortArray startOrderSeqSpec

    user specification for start_order_sequence
- size_t sequenceIndex

    sequence index for start{Rank,Order}SeqSpec

Additional Inherited Members

14.162.1 Detailed Description

Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.

The NonDMultilevelFunctionTrain class uses a set of function train (FT) expansions, one per model fidelity or resolution, to approximate the effect of parameter uncertainties on response functions of interest.

14.162.2 Constructor & Destructor Documentation

14.162.2.1 NonDMultilevelFunctionTrain (ProblemDescDB & *problem_db*, Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation using the ProblemDescDB.

References Dakota::abort_handler(), Response::active_set(), NonDMultilevelFunctionTrain::assign_allocation_control(), NonDExpansion::assign_discrepancy_mode(), NonDExpansion::assign_hierarchical_response_mode(), Model::assign_rep(), NonDMultilevelFunctionTrain::collocation_points(), ParallelLibrary::command_line_check(), NonDC3FunctionTrain::config_regression(), NonDExpansion::configure_expansion_orders(), NonDExpansion::construct_expansion_sampler(), Model::current_response(), ActiveSet::derivative_vector(), NonDExpansion::dimPrefSpec, ProblemDescDB::get_bool(), ProblemDescDB::get_iv(), ProblemDescDB::get_string(), ProblemDescDB::get_sza(), ProblemDescDB::get_ushort(), NonDC3FunctionTrain::importBuildPointsFile, NonDMultilevelFunctionTrain::initialize_u_space_model(), Iterator::iteratedModel, NonDExpansion::numSamplesOnModel, Iterator::outputLevel, Iterator::parallelLib, Iterator::probDescDB, Model::qoi(), NonDMultilevelFunctionTrain::random_seed(), NonDExpansion::randomSeedSeqSpec, NonDC3FunctionTrain::regression_size(), NonDC3FunctionTrain::resolve_inputs(), NonDMultilevelFunctionTrain::sequenceIndex, and NonDExpansion::uSpaceModel.

14.162.2.2 ∼NonDMultilevelFunctionTrain ( )

destructor

```
This constructor is used for helper iterator instantiation on the fly
that employ regression.
```

NonDMultilevelFunctionTrain:: NonDMultilevelFunctionTrain(unsigned short method_name, Model& model, const SizetArray& colloc_pts_seq, const RealVector& dim_pref, Real colloc_ratio, const SizetArray& seed_seq, short u-_space_type, short refine_type, short refine_control, short covar_control, short ml_alloc_control, short ml_discrep, short rule_nest, short rule_growth, bool piecewise_basis, bool use_derivs, bool cv_flag, const String& import_-build_pts_file, unsigned short import_build_format, bool import_build_active_only): NonDC3FunctionTrain(method-_name, model, exp_coeffs_approach, dim_pref, u_space_type, refine_type, refine_control, covar_control, colloc_-pts_seq, colloc_ratio, ml_alloc_control, ml_discrep, //rule_nest, rule_growth, piecewise_basis, use_derivs, 0, cv_-flag), expOrderSeqSpec(exp_order_seq), sequenceIndex(0) { randomSeedSeqSpec = seed_seq;

assign_discrepancy_mode(); assign_hierarchical_response_mode();

Resolve settings

short data_order; resolve_inputs(uSpaceType, data_order);

Recast g(x) to G(u)

Model g_u_model; g_u_model.assign_rep(std::make_shared<ProbabilityTransformModel> (iteratedModel, u-SpaceType)); // retain dist bounds

Construct u_space_sampler

Iterator u_space_sampler; // evaluates truth model if (!config_regression(collocation_points(), regression_-size(sequenceIndex), random_seed(), u_space_sampler, g_u_model)){ Cerr << "Error: incomplete configuration in NonDMultilevelFunctionTrain " << "constructor." << std::endl; abort_handler(METHOD_ERROR); }

Construct G-hat(u) = uSpaceModel

G-hat(u) uses an orthogonal polynomial approximation over the active/uncertain variables (using same view as iteratedModel/g_u_model: not the typical All view for DACE). No correction is employed. Note: for PCBDO with polynomials over {u}+{d}, change view to All. UShortArray start_orders; configure_expansion_orders(start-_order(), dimPrefSpec, start_orders); short corr_order = -1, corr_type = NO_CORRECTION; if (!import_build_pts_-file.empty()) pt_reuse = "all"; const ActiveSet& recast_set = g_u_model.current_response().active_set(); DFSModel: consume any QoI aggregation. Helper mode: support approx Hessians ShortArray asv(g_u_model.qoi(), 7); // TO DO: consider passing in data_mode ActiveSet pce_set(asv, recast_set.derivative_vector()); uSpaceModel.assign-_rep(std::make_shared<DataFitSurrModel>(u_space_sampler, g_u_model, pce_set, approx_type, start_orders, corr_type, corr_order, data_order, outputLevel, pt_reuse, import_build_pts_file, import_build_format, import_build-_active_only)); initialize_u_space_model();

Configure settings for ML allocation (requires uSpaceModel) assign_allocation_control();

no expansionSampler, no numSamplesOnExpansion }

14.162.3 Member Function Documentation

14.162.3.1 void increment_specification_sequence ( ) [protected], [virtual]

increment the input specification sequence and assign values

Default implementation redefined by Multilevel derived classes.

Reimplemented from NonDExpansion.

References NonDMultilevelFunctionTrain::assign_specification_sequence(), and NonDMultilevelFunctionTrain-::sequenceIndex.

14.162.3.2 void infer_pilot_sample (size_t *num_steps,* SizetArray & *delta_N_l*) [protected], [virtual]

Default implementation redefined by Multilevel derived classes.

Reimplemented from NonDExpansion.

References NonDExpansion::collocRatio, and NonDC3FunctionTrain::regression_size().

14.162.3.3 size_t regression_size (size_t *index*) [private]

return the regression size used for different refinement options; the index identifies the point in the specification sequence

This implementation differs from those in C3Approximation and SharedC3ApproxData in that they are used for sample initialization from specification sequences, prior to any adaptation. They pass current/max values to the general SharedC3ApproxData helper.

References NonDC3FunctionTrain::c3AdvancementType, NonDExpansion::configure_expansion_orders(), NonDExpansion::dimPrefSpec, NonDC3FunctionTrain::maxOrderSpec, NonDC3FunctionTrain::maxRankSpec, Analyzer::numContinuousVars, and SharedC3ApproxData::regression_size().

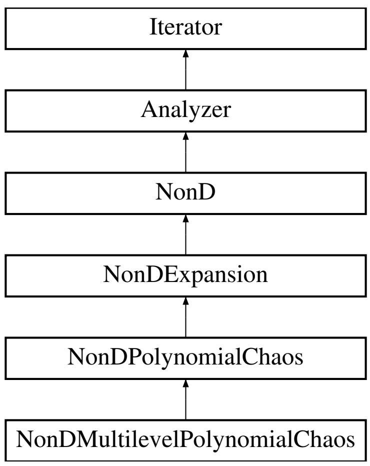
The documentation for this class was generated from the following files:

- NonDMultilevelFunctionTrain.hpp
- NonDMultilevelFunctionTrain.cpp

14.163 NonDMultilevelPolynomialChaos Class Reference

Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.

Inheritance diagram for NonDMultilevelPolynomialChaos:



Public Member Functions

- NonDMultilevelPolynomialChaos (ProblemDescDB &problem_db, Model &model)

    standard constructor
- NonDMultilevelPolynomialChaos (Model &model, short exp_coeffs_approach, const UShortArray &num_int-_seq, const RealVector &dim_pref, short u_space_type, short refine_type, short refine_control, short covar_-control, short ml_alloc_cntl, short ml_discrep, short rule_nest, short rule_growth, bool piecewise_basis, bool use_derivs)

    alternate constructor for numerical integration (tensor, sparse, cubature)

- NonDMultilevelPolynomialChaos (unsigned short method_name, Model &model, short exp_coeffs_approach, const UShortArray &exp_order_seq, const RealVector &dim_pref, const SizetArray &colloc_pts_seq, Real colloc_ratio, const SizetArray &seed_seq, short u_space_type, short refine_type, short refine_control, short covar_control, short ml_alloc_cntl, short ml_discrep, bool piecewise_basis, bool use_derivs, bool cv_flag, const String &import_build_pts_file, unsigned short import_build_format, bool import_build_active_only)

  alternate constructor for regression (least squares, CS, OLI)
- ∼NonDMultilevelPolynomialChaos ()

  destructor

Protected Member Functions

- void core_run ()

  perform a forward uncertainty propagation using PCE/SC methods
- void assign_specification_sequence ()

  assign the current values from the input specification sequence
- void increment_specification_sequence ()

  increment the input specification sequence and assign values
- size_t collocation_points () const

  return specification for number of collocation points (may be part of a sequence specification)
- int random_seed () const

  return specification for random seed (may be part of a sequence specification)
- int first_seed () const

  return first seed in sequence specification (defaults to random_seed())
- void initialize_ml_regression (size_t num_lev, bool &import_pilot)

  initializations for multilevel_regression()
- void infer_pilot_sample (size_t num_steps, SizetArray &delta_N_l)
- void increment_sample_sequence (size_t new_samp, size_t total_samp, size_t step)

  increment sequence in numSamplesOnModel for multilevel_regression()
- void compute_sample_increment (const RealVector &sparsity, const SizetArray &N_l, SizetArray &delta_N_l)

  compute delta_N_l for {RIP,RANK}_SAMPLING cases
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final statistics
- void assign_allocation_control ()

  assign defaults related to allocation control (currently for ML regression approaches)

Private Member Functions

- size_t **expansion_samples** (size_t index) const
- unsigned short **expansion_order** (size_t index) const
- unsigned short **quadrature_order** (size_t index) const
- unsigned short **sparse_grid_level** (size_t index) const
- size_t **expansion_samples** () const
- unsigned short **expansion_order** () const
- unsigned short **quadrature_order** () const
- unsigned short **sparse_grid_level** () const
- void update_from_specification (bool update_exp, bool update_sampler, bool update_from_ratio)

  perform specification updates (shared code from

Private Attributes

- UShortArray expOrderSeqSpec

    user specification for expansion_order (array for multifidelity)
- SizetArray expSamplesSeqSpec

    user specification for expansion_samples (array for multifidelity)
- UShortArray quadOrderSeqSpec

    user request of quadrature order
- UShortArray ssgLevelSeqSpec

    user request of sparse grid level
- size_t sequenceIndex

    sequence index for {...}SeqSpec

Additional Inherited Members

14.163.1 Detailed Description

Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.

The NonDMultilevelPolynomialChaos class uses a polynomial chaos expansion (PCE) approach to approximate the effect of parameter uncertainties on response functions of interest. It utilizes the OrthogPolyApproximation class to manage multiple types of orthogonal polynomials within a Wiener-Askey scheme to PCE. It supports PCE coefficient estimation via sampling, quadrature, point-collocation, and file import.

14.163.2 Constructor & Destructor Documentation

14.163.2.1 NonDMultilevelPolynomialChaos (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation using the ProblemDescDB.

References Dakota::abort_handler(), NonDMultilevelPolynomialChaos::assign_allocation_control(), NonDExpansion::assign_discrepancy_mode(), NonDExpansion::assign_hierarchical_response_mode(), Model::assign_rep(), NonDMultilevelPolynomialChaos::collocation_points(), ParallelLibrary::command_line_check(), NonDPolynomialChaos::config_expectation(), NonDPolynomialChaos::config_integration(), NonDPolynomialChaos::config_regression(), NonDExpansion::configure_expansion_orders(), NonDExpansion::construct_expansion_sampler(), NonDPolynomialChaos::cubIntSpec, ActiveSet::derivative_vector(), NonDExpansion::dimPrefSpec, ProblemDescDB::get_bool(), ProblemDescDB::get_iv(), ProblemDescDB::get_real(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), ProblemDescDB::get_sza(), ProblemDescDB::get_usa(), ProblemDescDB::get_ushort(), NonDPolynomialChaos::importBuildPointsFile, NonDPolynomialChaos::initialize_u_space_model(), Iterator::iteratedModel, NonDExpansion::numSamplesOnModel, Iterator::outputLevel, Iterator::parallelLib, Iterator::probDescDB, NonDMultilevelPolynomialChaos::random_seed(), NonDExpansion::randomSeedSeqSpec, NonDPolynomialChaos::resolve_inputs(), NonDExpansion::uSpaceModel, and NonDPolynomialChaos::uSpaceType.

14.163.2.2 NonDMultilevelPolynomialChaos (Model & *model,* short *exp_coeffs_approach,* const UShortArray & *num_int_seq,* const RealVector & *dim_pref,* short *u_space_type,* short *refine_type,* short *refine_control,* short *covar_control,* short *ml_alloc_control,* short *ml_discrep,* short *rule_nest,* short *rule_growth,* bool *piecewise_basis,* bool *use_derivs*)

alternate constructor for numerical integration (tensor, sparse, cubature)

This constructor is used for helper iterator instantiation on the fly that employ numerical integration (quadrature, sparse grid, cubature).

References Dakota::abort_handler(), Response::active_set(), NonDMultilevelPolynomialChaos::assign_allocation_control(), NonDExpansion::assign_discrepancy_mode(), NonDExpansion::assign_hierarchical_response_mode(), Model::assign_rep(), NonDPolynomialChaos::config_integration(), NonDPolynomialChaos::cubIntSpec, Model::current_response(), ActiveSet::derivative_vector(), NonDPolynomialChaos::initialize_u_space_model(), Iterator::iteratedModel, Iterator::outputLevel, Model::qoi(), NonDMultilevelPolynomialChaos::quadOrderSeqSpec, NonDPolynomialChaos::resolve_inputs(), NonDMultilevelPolynomialChaos::sequenceIndex, NonDMultilevelPolynomialChaos::ssgLevelSeqSpec, NonDExpansion::uSpaceModel, and NonDPolynomialChaos::uSpaceType.

14.163.2.3 NonDMultilevelPolynomialChaos (unsigned short *method_name,* Model & *model,* short *exp_coeffs_approach,* const UShortArray & *exp_order_seq,* const RealVector & *dim_pref,* const SizetArray & *colloc_pts_seq,* Real *colloc_ratio,* const SizetArray & *seed_seq,* short *u_space_type,* short *refine_type,* short *refine_control,* short *covar_control,* short *ml_alloc_control,* short *ml_discrep,* bool *piecewise_basis,* bool *use_derivs,* bool *cv_flag,* const String & *import_build_pts_file,* unsigned short *import_build_format,* bool *import_build_active_only*)

alternate constructor for regression (least squares, CS, OLI)

This constructor is used for helper iterator instantiation on the fly that employ regression (least squares, CS, OLI).

References Response::active_set(), NonDMultilevelPolynomialChaos::assign_allocation_control(), NonDExpansion::assign_discrepancy_mode(), NonDExpansion::assign_hierarchical_response_mode(), Model::assign_rep(), NonDMultilevelPolynomialChaos::collocation_points(), NonDPolynomialChaos::config_regression(), NonDExpansion::configure_expansion_orders(), Model::current_response(), ActiveSet::derivative_vector(), NonDExpansion::dimPrefSpec, NonDPolynomialChaos::initialize_u_space_model(), Iterator::iteratedModel, Iterator::outputLevel, Model::qoi(), NonDMultilevelPolynomialChaos::random_seed(), NonDExpansion::randomSeedSeqSpec, NonDPolynomialChaos::resolve_inputs(), NonDExpansion::uSpaceModel, and NonDPolynomialChaos::uSpaceType.

14.163.3 Member Function Documentation

14.163.3.1 void increment_specification_sequence ( ) [protected], [virtual]

increment the input specification sequence and assign values

Default implementation redefined by Multilevel derived classes.

Reimplemented from NonDExpansion.

References Dakota::abort_handler(), NonDExpansion::collocPtsSeqSpec, NonDExpansion::expansionCoeffsApproach, NonDMultilevelPolynomialChaos::expOrderSeqSpec, NonDMultilevelPolynomialChaos::expSamplesSeqSpec, Iterator::iterator_rep(), NonDExpansion::numSamplesOnModel, NonDMultilevelPolynomialChaos::quadOrderSeqSpec, NonDExpansion::randomSeedSeqSpec, NonDMultilevelPolynomialChaos::sequenceIndex, NonDMultilevelPolynomialChaos::ssgLevelSeqSpec, Model::subordinate_iterator(), NonDMultilevelPolynomialChaos::update_from_specification(), and NonDExpansion::uSpaceModel.

14.163.3.2 void infer_pilot_sample (size_t *num_steps,* SizetArray & *delta_N_l*) [protected], [virtual]

Default implementation redefined by Multilevel derived classes.

Reimplemented from NonDExpansion.

References NonDExpansion::collocRatio, NonDExpansion::configure_expansion_orders(), NonDExpansion::dimPrefSpec, NonDExpansion::expansionBasisType, and NonDExpansion::terms_ratio_to_samples().

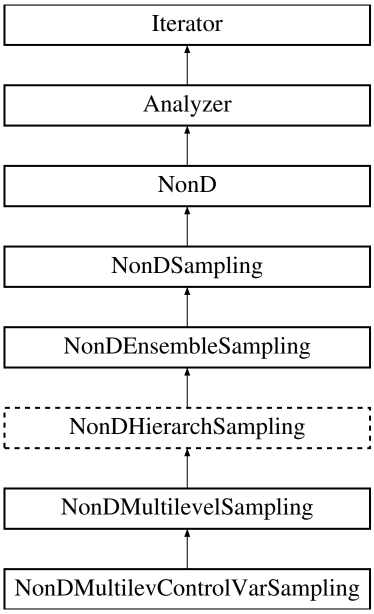
The documentation for this class was generated from the following files:

- NonDMultilevelPolynomialChaos.hpp
- NonDMultilevelPolynomialChaos.cpp

14.164 NonDMultilevelSampling Class Reference

Performs Multilevel Monte Carlo sampling for uncertainty quantification.

Inheritance diagram for NonDMultilevelSampling:



Public Member Functions

- NonDMultilevelSampling (ProblemDescDB &problem_db, Model &model)

  standard constructor
- ∼NonDMultilevelSampling ()

  destructor

Protected Member Functions

- void core_run ()
- void **print_variance_reduction** (std::ostream &s)
- void nested_response_mappings (const RealMatrix &primary_coeffs, const RealMatrix &secondary_coeffs)

  set primaryResponseCoefficients, secondaryResponseCoefficients within derived Iterators; Necessary for scalarization case in MLMC NonDMultilevelSampling to map scalarization in nested context
- void evaluate_ml_sample_increment (unsigned short step)

  helper that consolidates sequence advancement, sample generation, sample export, and sample evaluation
- void increment_ml_equivalent_cost (size_t new_N_l, Real lev_cost, Real ref_cost)

  increment the equivalent number of HF evaluations based on new model evaluations
- void compute_ml_estimator_variance (const RealMatrix &var_Y, const Sizet2DArray &num_Y, RealVector &ml_est_var)

  compute MLMC estimator variance from level QoI variances
- void recover_variance (const RealMatrix &moment_stats, RealVector &var_H)

  recover variance from raw moments
- void accumulate_ml_Ysums (IntRealMatrixMap &sum_Y, RealMatrix &sum_YY, size_t lev, SizetArray &num_Y)

  update accumulators for multilevel telescoping running sums using set of model evaluations within allResponses
- void accumulate_ml_Ysums (RealMatrix &sum_Y, RealMatrix &sum_YY, size_t lev, SizetArray &num_Y)

update accumulators for multilevel telescoping running sums using set of model evaluations within allResponses

- void accumulate_ml_Qsums (IntRealMatrixMap &sum_Q, size_t lev, SizetArray &num_Q)

    update running QoI sums for one model (sum_Q) using set of model evaluations within allResponses; used for level 0 from other accumulators

- Real variance_Ysum (Real sum_Y, Real sum_YY, size_t Nlq)

    compute variance scalar from sum accumulators

- void variance_Ysum (const Real ∗sum_Y, const Real ∗sum_YY, const SizetArray &N_l, Real ∗var_Y)

    compute variance column vec (all QoI for one level) from sum accumulators

- Real variance_Qsum (Real sum_Ql, Real sum_Qlm1, Real sum_QlQl, Real sum_QlQlm1, Real sum_Qlm1-Qlm1, size_t Nlq)

    compute variance from sum accumulators

- Real aggregate_variance_Ysum (const Real ∗sum_Y, const Real ∗sum_YY, const SizetArray &N_l)

    sum up variances across QoI (using sum_YY with means from sum_Y)

- Real aggregate_mse_Yvar (const Real ∗var_Y, const SizetArray &N_l)

    sum up Monte Carlo estimates for mean squared error (MSE) across QoI using discrepancy variances

- Real aggregate_mse_Ysum (const Real ∗sum_Y, const Real ∗sum_YY, const SizetArray &N_l)

    sum up Monte Carlo estimates for mean squared error (MSE) across QoI using discrepancy sums

- void ml_raw_moments (const RealMatrix &sum_H1, const RealMatrix &sum_H2, const RealMatrix &sum_H3, const RealMatrix &sum_H4, const Sizet2DArray &N_hf, size_t start, size_t end, RealMatrix &ml_raw_mom)

    accumulate ML-only contributions (levels with no CV) to raw moments

- void configure_indices (unsigned short group, unsigned short form, size_t lev, short seq_type)

    manage response mode and active model key from {group,form,lev} triplet. seq_type defines the active dimension for a 1D model sequence.

- void configure_indices (size_t group, size_t form, size_t lev, short seq_type)

    convert group and form and call overload

- Real level_cost (const RealVector &cost, size_t step)

    return (aggregate) level cost

Protected Attributes

- RealVector estVar

    final estimator variance for output in print_variance_reduction()

Private Types

- enum { **COV_BOOTSTRAP**, **COV_PEARSON**, **COV_CORRLIFT** }

Private Member Functions

- void multilevel_mc_Qsum ()

    Perform multilevel Monte Carlo across the discretization levels for a particular model form using QoI accumulators (sum_Q)

- void multilevel_mc_offline_pilot ()

    Qsum approach using a pilot sample treated as separate offline cost.

- void multilevel_mc_pilot_projection ()

    Qsum approach projecting estimator performance from a pilot sample.

- void evaluate_levels (IntRealMatrixMap &sum_Ql, IntRealMatrixMap &sum_Qlm1, IntIntPairRealMatrixMap &sum_QlQlm1, RealVector &cost, Sizet2DArray &N_pilot, Sizet2DArray &N_online, SizetArray &delta_N_l, RealMatrix &var_Y, RealMatrix &var_qoi, RealVector &eps_sq_div_2, bool increment_cost, bool pilot_estvar)

    helper for shared code among offline-pilot and pilot-projection modes

- void initialize_ml_Qsums (IntRealMatrixMap &sum_Ql, IntRealMatrixMap &sum_Qlm1, IntIntPairRealMatrixMap &sum_QlQlm1, size_t num_lev)

  initialize the ML accumulators for computing means, variances, and covariances across fidelity levels
- void reset_ml_Qsums (IntRealMatrixMap &sum_Ql, IntRealMatrixMap &sum_Qlm1, IntIntPairRealMatrixMap &sum_QlQlm1)

  reset existing ML accumulators to zero for all keys
- void store_evaluations (const size_t step)

  adds the response evaluations for the current step to levQoisamplesmatrixMap.
- void accumulate_ml_Qsums (IntRealMatrixMap &sum_Ql, IntRealMatrixMap &sum_Qlm1, IntIntPairRealMatrixMap &sum_QlQlm1, size_t lev, SizetArray &num_Q)

  update running QoI sums for two models (sum_Ql, sum_Qlm1) using set of model evaluations within allResponses
- void **compute_ml_equivalent_cost** (const SizetArray &raw_N_l, const RealVector &cost)
- void compute_error_estimates (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const Sizet2DArray &num_Q)

  populate finalStatErrors for MLMC based on Q sums
- void update_projected_samples (const SizetArray &delta_N_l, Sizet2DArray &N_l, const RealVector &cost)

  for pilot projection, advance the sample counts and aggregate cost based on projected rather than actual samples
- Real **var_lev_l** (Real sum_Ql, Real sum_Qlm1, Real sum_QlQl, Real sum_Qlm1Qlm1, size_t Nlq)
- void aggregate_variance_target_Qsum (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_-Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const Sizet2DArray &N_l, const size_t step, RealMatrix &agg_var_qoi)

  sum up variances for QoI (using sum_YY with means from sum_Y) based on allocation target
- Real variance_mean_Qsum (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const Sizet2DArray &N_l, const size_t step, const size_t qoi)

  wrapper for variance_Qsum
- Real aggregate_variance_Qsum (const Real ∗sum_Ql, const Real ∗sum_Qlm1, const Real ∗sum_QlQl, const Real ∗sum_QlQlm1, const Real ∗sum_Qlm1Qlm1, const SizetArray &N_l, const size_t lev)

  sum up variances across QoI for given level
- Real variance_Qsum (const Real ∗sum_Ql, const Real ∗sum_Qlm1, const Real ∗sum_QlQl, const Real ∗sum_QlQlm1, const Real ∗sum_Qlm1Qlm1, const SizetArray &N_l, const size_t lev, const size_t qoi)

  evaluate variance for given level and QoI (using sum_YY with means from sum_Y)
- void variance_Qsum (const Real ∗sum_Ql, const Real ∗sum_Qlm1, const Real ∗sum_QlQl, const Real ∗sum-_QlQlm1, const Real ∗sum_Qlm1Qlm1, const SizetArray &N_l, const size_t lev, Real ∗var_Yl)

  evaluate variances for given level across set of QoI
- Real variance_variance_Qsum (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const Sizet2DArray &N_l, const size_t step, const size_t qoi)

  wrapper for var_of_var_ml
- Real variance_sigma_Qsum (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const Sizet2DArray &N_l, const size_t step, const size_t qoi)

  wrapper for var_of_sigma_ml
- Real variance_scalarization_Qsum (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const Sizet2DArray &N_l, const size_t step, const size_t qoi)

  wrapper for var_of_scalarization_ml
- void aggregate_mse_target_Qsum (RealMatrix &agg_var_qoi, const Sizet2DArray &N_l, const size_t step, RealVector &estimator_var0_qoi)

  sum up Monte Carlo estimates for mean squared error (MSE) for QoI using discrepancy sums based on allocation target
- void set_convergence_tol (const RealVector &estimator_var0_qoi, const RealVector &cost, RealVector &eps-_sq_div_2_qoi)

  compute epsilon^2/2 term for each qoi based on reference estimator_var0 and relative convergence tolereance
- void compute_sample_allocation_target (const RealMatrix &var_qoi, const RealVector &cost, const Sizet2D-Array &N_l, SizetArray &delta_N_l)

  compute sample allocation delta based on a budget constraint

- void compute_sample_allocation_target (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_-Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const RealVector &eps_sq_div_2_in, const RealMatrix &var_qoi, const RealVector &cost, const Sizet2DArray &N_pilot, const Sizet2DArray &N_online, SizetArray &delta_N_l)

    compute sample allocation delta based on current samples and based on allocation target. Single allocation target for each qoi, aggregated using max operation.
- void **compute_moments** (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const Sizet2DArray &N_l)
- void **assign_static_member** (const Real &conv_tol, size_t &qoi, const size_t &qoi_aggregation, const size_t &num_functions, const RealVector &level_cost_vec, const IntRealMatrixMap &sum_Ql, const IntRealMatrix-Map &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const RealVector &pilot_samples, const RealMatrix &scalarization_response_mapping)
- void **assign_static_member_problem18** (Real &var_L_exact, Real &var_H_exact, Real &mu_four_L_exact, Real &mu_four_H_exact, Real &Ax, RealVector &level_cost_vec) const

Static Private Member Functions

- static Real variance_Ysum_static (Real sum_Y, Real sum_YY, size_t Nlq_pilot, size_t Nlq, bool compute_-gradient, Real &grad)

    compute variance from sum accumulators necessary for sample allocation optimization
- static Real variance_Qsum_static (Real sum_Ql, Real sum_Qlm1, Real sum_QlQl, Real sum_QlQlm1, Real sum_Qlm1Qlm1, size_t Nlq_pilot, size_t Nlq, bool compute_gradient, Real &grad)

    compute variance from sum accumulators necessary for sample allocation optimization
- static Real **var_lev_l_static** (Real sum_Ql, Real sum_Qlm1, Real sum_QlQl, Real sum_Qlm1Qlm1, size_t Nlq_pilot, size_t Nlq, bool compute_gradient, Real &grad)
- static Real **compute_bootstrap_covariance** (const size_t step, const size_t qoi, const IntRealMatrixMap &lev_qoisamplematrix_map, const Real N, const bool compute_gradient, Real &grad, int ∗seed)
- static Real **compute_cov_mean_sigma** (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum-_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const size_t Nlq_pilot, const Real Nlq, const size_t qoi, const size_t lev, const bool compute_gradient, Real &grad_g)
- static RealVector **compute_cov_mean_sigma_fd** (const IntRealMatrixMap &sum_Ql, const IntRealMatrix-Map &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const size_t Nlq_pilot, const Real Nlq, const size_t qoi, const size_t lev)
- static Real **compute_mean** (const RealVector &samples)
- static Real **compute_mean** (const RealVector &samples, const bool compute_gradient, Real &grad)
- static Real **compute_mean** (const RealVector &samples, const Real N)
- static Real **compute_mean** (const RealVector &samples, const Real N, const bool compute_gradient, Real &grad)
- static Real **compute_std** (const RealVector &samples)
- static Real **compute_std** (const RealVector &samples, const bool compute_gradient, Real &grad)
- static Real **compute_std** (const RealVector &samples, const Real N)
- static Real **compute_std** (const RealVector &samples, const Real N, const bool compute_gradient, Real &grad)
- static Real **compute_cov** (const RealVector &samples_X, const RealVector &samples_hat)
- static Real unbiased_mean_product_pair (const Real sumQ1, const Real sumQ2, const Real sumQ1Q2, const size_t Nlq)

    compute the unbiased product of two sampling means
- static Real unbiased_mean_product_triplet (const Real sumQ1, const Real sumQ2, const Real sumQ3, const Real sumQ1Q2, const Real sumQ1Q3, const Real sumQ2Q3, const Real sumQ1Q2Q3, const size_t Nlq)

    compute the unbiased product of three sampling means
- static Real unbiased_mean_product_pairpair (const Real sumQ1, const Real sumQ2, const Real sumQ1Q2, const Real sumQ1sq, const Real sumQ2sq, const Real sumQ1sqQ2, const Real sumQ1Q2sq, const Real sumQ1sqQ2sq, const size_t Nlq)

    compute the unbiased product of two pairs of products of sampling means

- static Real **var_of_var_ml_l0** (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const size_t Nlq_pilot, const Real Nlq, const size_t qoi, const bool compute_gradient, Real &grad_g)
- static Real **var_of_var_ml_lmax** (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const size_t Nlq_pilot, const Real Nlq, const size_t qoi, const bool compute_gradient, Real &grad_g)
- static Real **var_of_var_ml_l** (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const size_t Nlq_pilot, const Real Nlq, const size_t qoi, const size_t lev, const bool compute_gradient, Real &grad_g)
- static Real **compute_cov_meanl_varlmone** (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const size_t Nlq_pilot, const Real Nlq, const size_t qoi, const size_t lev, const bool compute_gradient, Real &grad_g)
- static Real **compute_cov_meanlmone_varl** (const IntRealMatrixMap &sum_Ql, const IntRealMatrixMap &sum_Qlm1, const IntIntPairRealMatrixMap &sum_QlQlm1, const size_t Nlq_pilot, const Real Nlq, const size_t qoi, const size_t lev, const bool compute_gradient, Real &grad_g)
- static Real **compute_grad_cov_meanl_vark** (const Real cov_mean_var, const Real var_of_var, const Real var_of_sigma, const Real grad_var_of_var, const Real grad_var_of_sigma, const Real Nlq)
- static void target_cost_objective_eval_optpp (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode)

  OPTPP definition.
- static void **target_cost_constraint_eval_optpp** (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
- static void **target_var_constraint_eval_optpp** (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
- static void **target_var_constraint_eval_logscale_optpp** (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
- static void **target_sigma_constraint_eval_optpp** (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
- static void **target_sigma_constraint_eval_logscale_optpp** (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
- static void **target_scalarization_constraint_eval_optpp** (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
- static void **target_scalarization_constraint_eval_logscale_optpp** (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
- static void **target_var_objective_eval_optpp** (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode)
- static void **target_var_objective_eval_logscale_optpp** (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode)
- static void **target_sigma_objective_eval_optpp** (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode)
- static void **target_sigma_objective_eval_logscale_optpp** (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode)
- static void **target_scalarization_objective_eval_optpp** (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode)
- static void **target_scalarization_objective_eval_logscale_optpp** (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode)
- static void **target_scalarization_objective_eval_optpp_fd** (int mode, int n, const RealVector &x, double &f, int &result_mode)
- static void target_cost_objective_eval_npsol (int &mode, int &n, double ∗x, double &f, double ∗gradf, int &nstate)

  NPSOL definition (Wrapper using OPTPP implementation above under the hood)
- static void **target_cost_constraint_eval_npsol** (int &mode, int &m, int &n, int &ldJ, int ∗needc, double ∗x, double ∗g, double ∗grad_g, int &nstate)
- static void **target_var_constraint_eval_npsol** (int &mode, int &m, int &n, int &ldJ, int ∗needc, double ∗x, double ∗g, double ∗grad_g, int &nstate)

- static void **target_var_constraint_eval_logscale_npsol** (int &mode, int &m, int &n, int &ldJ, int *needc, double *x, double *g, double *grad_g, int &nstate)
- static void **target_sigma_constraint_eval_npsol** (int &mode, int &m, int &n, int &ldJ, int *needc, double *x, double *g, double *grad_g, int &nstate)
- static void **target_sigma_constraint_eval_logscale_npsol** (int &mode, int &m, int &n, int &ldJ, int *needc, double *x, double *g, double *grad_g, int &nstate)
- static void **target_scalarization_constraint_eval_npsol** (int &mode, int &m, int &n, int &ldJ, int *needc, double *x, double *g, double *grad_g, int &nstate)
- static void **target_scalarization_constraint_eval_logscale_npsol** (int &mode, int &m, int &n, int &ldJ, int *needc, double *x, double *g, double *grad_g, int &nstate)
- static void **target_var_objective_eval_npsol** (int &mode, int &n, double *x, double &f, double *gradf, int &nstate)
- static void **target_var_objective_eval_logscale_npsol** (int &mode, int &n, double *x, double &f, double *gradf, int &nstate)
- static void **target_sigma_objective_eval_npsol** (int &mode, int &n, double *x, double &f, double *gradf, int &nstate)
- static void **target_sigma_objective_eval_logscale_npsol** (int &mode, int &n, double *x, double &f, double *gradf, int &nstate)
- static void **target_scalarization_objective_eval_npsol** (int &mode, int &n, double *x, double &f, double *gradf, int &nstate)
- static void **target_scalarization_objective_eval_logscale_npsol** (int &mode, int &n, double *x, double &f, double *gradf, int &nstate)
- static void **target_var_constraint_eval_optpp_problem18** (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
- static void **target_sigma_constraint_eval_optpp_problem18** (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)
- static double **exact_var_of_var_problem18** (const RealVector &Nl)
- static double **exact_var_of_sigma_problem18** (const RealVector &Nl)

Private Attributes

- unsigned short **seq_index**
- short allocationTarget

    store the allocation_target input specification, prior to run-time Options right now:
- bool useTargetVarianceOptimizationFlag

    option to switch on numerical optimization for solution of sample alloation of allocationTarget Variance
- short qoiAggregation

    store the qoi_aggregation_norm input specification, prior to run-time Options right now:
- short convergenceTolType

    `store the convergence_tolerance_type input specification, prior to run-time`
    Options right now:
- short convergenceTolTarget

    store the convergence_tolerance_target input specification, prior to run-time Options right now:
- RealVector **convergenceTolVec**
- RealMatrix scalarizationCoeffs

    *"scalarization" response_mapping matrix applied to the mlmc sample allocation when a scalarization, i.e. alpha_1 * mean + alpha_2 * sigma, is the target.*
- RealMatrix NTargetQoi

    Helper data structure to store intermedia sample allocations.
- RealMatrix **NTargetQoiFN**
- IntRealMatrixMap **levQoisamplesmatrixMap**
- bool **storeEvals**
- int **bootstrapSeed**
- short **cov_approximation_type**

Additional Inherited Members

14.164.1 Detailed Description

Performs Multilevel Monte Carlo sampling for uncertainty quantification.

Multilevel Monte Carlo (MLMC) is a variance-reduction technique that utilitizes lower fidelity simulations that have response QoI that are correlated with the high-fidelity response QoI.

14.164.2 Constructor & Destructor Documentation

14.164.2.1 NonDMultilevelSampling (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDMultilevelSampling::allocationTarget, NonD::finalMomentsType, ProblemDescDB::get_rv(), Iterator::iteratedModel, Model::multifidelity_precedence(), Analyzer::numFunctions, Iterator::probDescDB, NonDMultilevelSampling::qoiAggregation, and NonDMultilevelSampling::scalarizationCoeffs.

14.164.3 Member Function Documentation

14.164.3.1 void core_run ( ) [protected], [virtual]

The primary run function manages the general case: a hierarchy of model forms (from the ordered model fidelities within a HierarchSurrModel), each of which may contain multiple discretization levels.

Reimplemented from Iterator.

References Dakota::abort_handler(), NonDMultilevelSampling::allocationTarget, NonD::configure_sequence(), Iterator::convergenceTol, NonDMultilevelSampling::multilevel_mc_offline_pilot(), NonDMultilevelSampling::multilevel_mc_pilot_projection(), NonDMultilevelSampling::multilevel_mc_Qsum(), Analyzer::numFunctions, NonDEnsembleSampling::numSteps, NonDEnsembleSampling::onlineCost, NonDEnsembleSampling::pilotMgmtMode, NonD::query_cost(), NonDMultilevelSampling::scalarizationCoeffs, NonDEnsembleSampling::secondaryIndex, NonDEnsembleSampling::sequenceCost, and NonDEnsembleSampling::sequenceType.

Referenced by NonDMultilevControlVarSampling::core_run().

14.164.3.2 void multilevel_mc_Qsum ( ) [private]

Perform multilevel Monte Carlo across the discretization levels for a particular model form using QoI accumulators (sum_Q)

```
This function performs MLMC on a model sequence, either defined by
model forms or discretization levels.
```

void NonDMultilevelSampling::multilevel_mc_Ysum() { Formulate as a coordinated progression towards convergence, where, e.g., time step is inferred from the spatial discretization (NOT an additional solution control) based on stability criteria, e.g. CFL condition. Can we reliably capture runtime estimates as part of pilot run w/i Dakota? Ultimately seems desirable to support either online or offline cost estimates, to allow more accurate resource allocation when possible or necessary (e.g., combustion processes with expense that is highly parameter dependent). model id_model = 'LF' simulation

point to state vars; ordered based on set values for h, delta-t

solution_level_control = 'dssiv1'

relative cost estimates in same order as state set values

–> re-sort into map keyed by increasing cost

solution_level_cost = 10 2 200

How to manage the set of MLMC statistics:

1. Simplest: proposal is to use the mean estimator to drive the algorithm, but carry along other estimates.
2. Later: could consider a refinement for converging the estimator of the variance after convergence of the mean estimator.

How to manage the vector of QoI:

1. Worst case: select N_l based only on QoI w/ highest total variance from pilot run –> fix for all levels and don't allow switching across major iterations (possible oscillation? Or simple overlay of resolution reqmts?)
2. Better: select N_l based on convergence in aggregated variance.

Allow either model forms or discretization levels, but not both size_t form, lev; bool multilev = (sequenceType == Pecos::RESOLUTION_LEVEL_SEQUENCE), budget_constrained = (maxFunctionEvals != SZ_MAX); either lev varies and form is fixed, or vice versa: size_t& step = (multilev) ? lev : form; if (multilev) form = secondaryIndex; else lev = secondaryIndex;

retrieve cost estimates across soln levels for a particular model form RealVector agg_var(numSteps); Real eps_sq_div_2, sum_sqrt_var_cost, agg_estvar0 = 0., lev_cost, budget, ref_cost = sequenceCost[numSteps-1]; // HF cost (1 level)

if (budget_constrained) budget = (Real)maxFunctionEvals ∗ ref_cost; For moment estimation, we accumulate telescoping sums for Q^i using discrepancies Yi = Q^i_{lev} - Q^i_{lev-1} (sum_Y[i] for i=1:4). For computing N_l from estimator variance, we accumulate square of Y1 estimator (YY[i] = (Y^i)^2 for i=1). IntRealMatrixMap sum_Y; RealMatrix sum_YY(numFunctions, numSteps); initialize_ml_Ysums(sum_Y, numSteps); RealMatrix var_Y(numFunctions, numSteps, false);

Initialize for pilot sample SizetArray delta_N_l; load_pilot_sample(pilotSamples, numSteps, delta_N_l);

Sizet2DArray& N_l = NLev[form]; // slice only valid for ML define a new 2D array and then post back to NLev at end Sizet2DArray N_l(numSteps); for (step=0; step<numSteps; ++step) N_l[step].assign(numFunctions, 0);

now converge on sample counts per level (N_l) while (Pecos::l1_norm(delta_N_l) && mlmfIter <= maxIterations) {

sum_sqrt_var_cost = 0.; for (step=0; step<numSteps; ++step) { // step is reference to lev

configure_indices(step, form, lev, sequenceType); lev_cost = level_cost(sequenceCost, step); // raw cost (not equiv HF)

set the number of current samples from the defined increment numSamples = delta_N_l[step];

aggregate variances across QoI for estimating N_l (justification: for independent QoI, sum of QoI variances = variance of QoI sum) Real& agg_var_l = agg_var[step]; // carried over from prev iter if no samp if (numSamples) {

assign sequence, get samples, export, evaluate evaluate_ml_sample_increment(step);

process allResponses: accumulate new samples for each qoi and update number of successful samples for each QoI accumulate_ml_Ysums(sum_Y, sum_YY, lev, N_l[step]); increment_ml_equivalent_cost(numSamples, lev_cost, ref_cost);

compute estimator variance from current sample accumulation: variance_Ysum(sum_Y[1][step], sum_YY[step], N_l[step], var_Y[step]); agg_var_l = sum(var_Y[lev], numFunctions); }

sum_sqrt_var_cost += std::sqrt(agg_var_l ∗ lev_cost); MSE reference is MLMC with pilot sample, prior to any N_l adaptation: if (mlmfIter == 0 && !budget_constrained) agg_estvar0 += aggregate_mse_Yvar(var_Y[step], N_l[step]); } compute epsilon target based on relative tolerance: total MSE = eps^2 which is equally apportioned (eps^2 / 2) among residual bias and estimator variance (var_Y_l / N_l). Since we usually do not know the bias error, we compute an initial estimator variance from MLMC on the pilot sample and then seek to reduce it by a relative_factor

<= 1. if (mlmfIter == 0) { MLMC estimator variance for final estvar reporting is not aggregated compute_ml_-estimator_variance(var_Y, N_l, estVarIter0);//numHIter0=numH; compute eps^2 / 2 = aggregated estvar0 * rel tol if (!budget_constrained) // eps^2 / 2 = estvar0 * rel tol eps_sq_div_2 = agg_estvar0 * convergenceTol; }

update sample targets based on latest variance estimates Real N_target, fact = (budget_constrained) ? budget / sum_sqrt_var_cost : // budget constraint sum_sqrt_var_cost / eps_sq_div_2; // error balance constraint for (step=0; step<numSteps; ++step) { Equation 3.9 in CTR Annual Research Briefs: "A multifidelity control variate approach for the multilevel Monte Carlo technique," Geraci, Eldred, Iaccarino, 2015. N_target = std::sqrt(agg_var[step]/level-_cost(sequenceCost, step)) * fact; delta_N_l[step] = one_sided_delta(average(N_l[step]), N_target); } ++mlmfIter; Cout << "\nMLMC iteration " << mlmfIter << " sample increments:\n" << delta_N_l << std::endl; }

switch (pilotMgmtMode) { case ONLINE_PILOT: case OFFLINE_PILOT: { aggregate expected value of estimators for Y, Y^2, Y^3, Y^4. Final expectation is sum of expectations from telescopic sum. Note: raw moments have no bias correction (no additional variance from estimated center). RealMatrix Q_raw_mom(numFunctions, 4); ml-_raw_moments(sum_Y[1], sum_Y[2], sum_Y[3], sum_Y[4], N_l, 0, numSteps, Q_raw_mom); convert_moments(-Q_raw_mom, momentStats); // raw to final (central or std) recover_variance(momentStats, varH); break; } case PILOT_PROJECTION: update_projected_samples(delta_N_l, N_l, sequenceCost); break; }

compute_ml_estimator_variance(var_Y, N_l, estVar); avgEstVar = average(estVar); post final N_l back to NLev (needed for final eval summary) inflate_final_samples(N_l, multilev, secondaryIndex, NLev); }This function performs "geometrical" MLMC on a single model form with multiple discretization levels.

References NonDEnsembleSampling::average(), NonDEnsembleSampling::avgEstVar, NonDMultilevelSampling-::compute_error_estimates(), NonDMultilevelSampling::compute_ml_estimator_variance(), NonDMultilevel-Sampling::estVar, NonDMultilevelSampling::evaluate_levels(), NonDEnsembleSampling::finalStatsType, NonD-::inflate_final_samples(), NonDMultilevelSampling::initialize_ml_Qsums(), NonD::load_pilot_sample(), Iterator-::maxIterations, NonDEnsembleSampling::mlmfIter, NonD::momentStats, NonDEnsembleSampling::NLev, Non-DEnsembleSampling::numSteps, NonDEnsembleSampling::pilotSamples, NonDMultilevelSampling::recover_-variance(), NonDEnsembleSampling::secondaryIndex, NonDEnsembleSampling::sequenceCost, NonDEnsemble-Sampling::sequenceType, and NonDEnsembleSampling::varH.

Referenced by NonDMultilevelSampling::core_run().

14.164.3.3 Real variance_scalarization_Qsum (const IntRealMatrixMap & *sum_Ql,* const IntRealMatrixMap & *sum_Qlm1,* const IntIntPairRealMatrixMap & *sum_QlQlm1,* const Sizet2DArray & *N_l,* const size_t *step,* const size_t *qoi*) [private]

wrapper for var_of_scalarization_ml

For TARGET_SCALARIZATION we have the special case that we can also combine scalarization over multiple qoi This is respresented in the scalarization response mapping stored in scalarizationCoeffs This is for now neglecting cross terms for covariance terms inbetween different qois, e.g. V[mu_1 + 2 sigma_1 + 3 mu_2] = V[mu_1] + V[2 sigma_1] + 2 Cov[mu_1, 2 sigma_1] + V[3 mu_2] + 2 Cov[2 mu_1, 3 mu_2] + 2 Cov[2 sigma_1, 3 mu_2] V[mu_1] + V[2 sigma_1] + 2 Cov[mu_1, 2 sigma_1] + V[3 mu_2] (What we do)

References NonDEnsembleSampling::check_negative(), Analyzer::numFunctions, NonDMultilevelSampling-::scalarizationCoeffs, NonDMultilevelSampling::variance_mean_Qsum(), and NonDMultilevelSampling::variance_-sigma_Qsum().

Referenced by NonDMultilevelSampling::aggregate_variance_target_Qsum().

14.164.4 Member Data Documentation

14.164.4.1 short allocationTarget [private]

store the allocation_target input specification, prior to run-time Options right now:

- Mean = First moment (Mean)
- Variance = Second moment (Variance or standard deviation depending on moments central or standard)

Referenced by NonDMultilevelSampling::aggregate_variance_target_Qsum(), NonDMultilevelSampling::compute-_sample_allocation_target(), NonDMultilevelSampling::core_run(), and NonDMultilevelSampling::NonDMultilevel-Sampling().

14.164.4.2 short qoiAggregation [private]

store the qoi_aggregation_norm input specification, prior to run-time Options right now:

- sum = aggregate the variance over all QoIs, compute samples from that
- max = take maximum sample allocation over QoIs for each level

Referenced by NonDMultilevelSampling::compute_sample_allocation_target(), and NonDMultilevelSampling::Non-DMultilevelSampling().

14.164.4.3 short convergenceTolType [private]

```
store the convergence_tolerance_type input specification, prior to run-time
```

Options right now:

- relative = computes reference tolerance in first iteration and sets convergence_tolerance as reference tolerance $*$ convergence_tol
- absolute = sets convergence tolerance from input

Referenced by NonDMultilevelSampling::set_convergence_tol().

14.164.4.4 short convergenceTolTarget [private]

store the convergence_tolerance_target input specification, prior to run-time Options right now:

- variance_constraint = minimizes cost for equality constraint on variance of estimator (rhs of constraint from convergenceTol)
- cost_constraint = minizes variance of estimator for equality constraint on cost (rhs of constraint from convergenceTol)

Referenced by NonDMultilevelSampling::compute_sample_allocation_target(), and NonDMultilevelSampling::set_-convergence_tol().

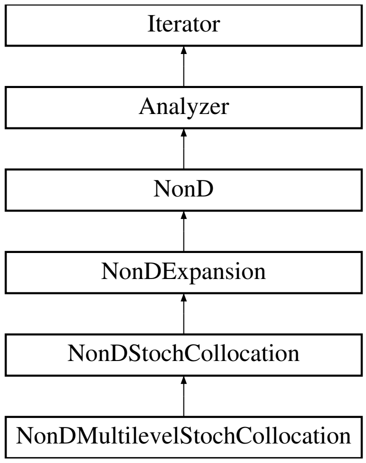
The documentation for this class was generated from the following files:

- NonDMultilevelSampling.hpp
- NonDMultilevelSampling.cpp

14.165 NonDMultilevelStochCollocation Class Reference

Nonintrusive stochastic collocation approaches to uncertainty quantification.

Inheritance diagram for NonDMultilevelStochCollocation:



Public Member Functions

- NonDMultilevelStochCollocation (ProblemDescDB &problem_db, Model &model)

  standard constructor
- NonDMultilevelStochCollocation (Model &model, short exp_coeffs_approach, const UShortArray &num_int_-seq, const RealVector &dim_pref, short u_space_type, short refine_type, short refine_control, short covar_-control, short ml_alloc_cntl, short ml_discrep, short rule_nest, short rule_growth, bool piecewise_basis, bool use_derivs)

  alternate constructor
- ∼NonDMultilevelStochCollocation ()

  destructor
- bool resize ()

  reinitializes iterator based on new variable size

Protected Member Functions

- void core_run ()

  perform a forward uncertainty propagation using PCE/SC methods
- int random_seed () const

  return specification for random seed (may be part of a sequence specification)
- int first_seed () const

  return first seed in sequence specification (defaults to random_seed())
- void assign_specification_sequence ()

  assign the current values from the input specification sequence
- void increment_specification_sequence ()

  increment the input specification sequence and assign values
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final statistics

Private Attributes

- UShortArray quadOrderSeqSpec

  user request of quadrature order
- UShortArray ssgLevelSeqSpec

  user request of sparse grid level
- size_t sequenceIndex

  sequence index for {quadOrder,ssgLevel}SeqSpec

Additional Inherited Members

14.165.1 Detailed Description

Nonintrusive stochastic collocation approaches to uncertainty quantification.

The NonDMultilevelStochCollocation class uses a stochastic collocation (SC) approach to approximate the effect of parameter uncertainties on response functions of interest. It utilizes the InterpPolyApproximation class to manage multidimensional Lagrange polynomial interpolants.

14.165.2 Constructor & Destructor Documentation

14.165.2.1 NonDMultilevelStochCollocation (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation using the ProblemDescDB.

References Response::active_set(), NonDExpansion::assign_discrepancy_mode(), NonDExpansion::assign_hierarchical_response_mode(), Model::assign_rep(), ParallelLibrary::command_line_check(), NonDStochCollocation::config_approximation_type(), NonDStochCollocation::config_integration(), NonDExpansion::construct_expansion_sampler(), Model::current_response(), ActiveSet::derivative_vector(), ProblemDescDB::get_bool(), ProblemDescDB::get_iv(), ProblemDescDB::get_rv(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), ProblemDescDB::get_ushort(), NonDStochCollocation::initialize_u_space_model(), Iterator::iteratedModel, NonDExpansion::numSamplesOnModel, Iterator::outputLevel, Iterator::parallelLib, Iterator::probDescDB, Model::qoi(), NonDMultilevelStochCollocation::quadOrderSeqSpec, NonDStochCollocation::resolve_inputs(), NonDMultilevelStochCollocation::sequenceIndex, NonDMultilevelStochCollocation::ssgLevelSeqSpec, and NonDExpansion::uSpaceModel.

14.165.2.2 NonDMultilevelStochCollocation (Model & *model,* short *exp_coeffs_approach,* const UShortArray & *num_int_seq,* const RealVector & *dim_pref,* short *u_space_type,* short *refine_type,* short *refine_control,* short *covar_control,* short *ml_alloc_cntl,* short *ml_discrep,* short *rule_nest,* short *rule_growth,* bool *piecewise_basis,* bool *use_derivs*)

alternate constructor

This constructor is used for helper iterator instantiation on the fly.

References Response::active_set(), NonDExpansion::assign_discrepancy_mode(), NonDExpansion::assign_hierarchical_response_mode(), Model::assign_rep(), NonDStochCollocation::config_approximation_type(), NonDStochCollocation::config_integration(), Model::current_response(), ActiveSet::derivative_vector(), NonDExpansion::expansionCoeffsApproach, NonDStochCollocation::initialize_u_space_model(), Iterator::iteratedModel, Iterator::outputLevel, Model::qoi(), NonDMultilevelStochCollocation::quadOrderSeqSpec, NonDStochCollocation::resolve_inputs(), NonDMultilevelStochCollocation::sequenceIndex, NonDMultilevelStochCollocation::ssgLevelSeqSpec, and NonDExpansion::uSpaceModel.

14.165.3 Member Function Documentation

14.165.3.1 void increment_specification_sequence ( ) [protected], [virtual]

increment the input specification sequence and assign values

Default implementation redefined by Multilevel derived classes.

Reimplemented from NonDExpansion.

References Dakota::abort_handler(), NonDExpansion::expansionCoeffsApproach, Iterator::iterator_rep(), NonDMultilevelStochCollocation::quadOrderSeqSpec, NonDMultilevelStochCollocation::sequenceIndex, NonDMultilevelStochCollocation::ssgLevelSeqSpec, Model::subordinate_iterator(), and NonDExpansion::uSpaceModel.

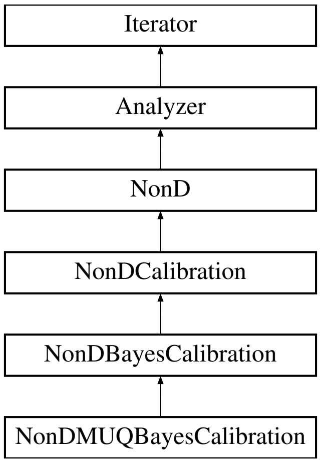
The documentation for this class was generated from the following files:

- NonDMultilevelStochCollocation.hpp
- NonDMultilevelStochCollocation.cpp

14.166 NonDMUQBayesCalibration Class Reference

Dakota interface to MUQ (MIT Uncertainty Quantification) library.

Inheritance diagram for NonDMUQBayesCalibration:



Public Member Functions

- NonDMUQBayesCalibration (ProblemDescDB &problem_db, Model &model)

  standard constructor
- ∼NonDMUQBayesCalibration ()

  destructor

Protected Member Functions

- void calibrate ()
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final iterator results
- void print_variables (std::ostream &s, const RealVector &c_vars)

  convenience function to print calibration parameters, e.g., for MAP / best parameters
- void cache_chain ()

  cache the chain to acceptanceChain and acceptedFnVals
- void log_best ()

  log at most batchSize best chain points into bestSamples
- void specify_prior () override

  initialize the MUQ parameter space, min, max, initial, domain, and prior define solver options, likelihood callback, posterior RV, and inverse problem
- void **specify_likelihood** () override
- void **init_bayesian_solver** () override
- void **specify_posterior** () override
- void init_proposal_covariance ()

  set the proposal covariance matrix

- void prior_proposal_covariance ()

  use covariance of prior distribution for setting proposal covariance
- void user_proposal_covariance (const String &input_fmt, const RealVector &cov_data, const String &cov_-filename)

  set proposal covariance from user-provided diagonal or matrix
- void **validate_proposal** ()

Protected Attributes

- std::shared_ptr
  < muq::Modeling::WorkGraph > **workGraph**
- std::shared_ptr
  < muq::Modeling::IdentityOperator > **parameterPtr**
- std::shared_ptr
  < muq::Modeling::Distribution > **distPtr**
- std::shared_ptr
  < muq::Modeling::DensityProduct > **posteriorPtr**
- std::shared_ptr< MUQLikelihood > **MUQLikelihoodPtr**
- std::shared_ptr< MUQPrior > **MUQPriorPtr**
- std::shared_ptr
  < muq::SamplingAlgorithms::SingleChainMCMC > **mcmc**
- std::shared_ptr
  < muq::SamplingAlgorithms::SampleCollection > **samps**
- String mcmcType

  MCMC type ("dram" or "delayed_rejection" or "adaptive_metropolis" or "metropolis_hastings" or "multilevel", within QUESO)
- unsigned int numBestSamples

  number of best samples (max log_posterior values) to keep
- Eigen::MatrixXd proposalCovMatrix

  proposal covariance for MCMC
- double priorPropCovMult

  optional multiplier to scale prior-based proposal covariance
- RealVector init_point

  initial guess (user-specified or default initial values)

Static Protected Attributes

- static NonDMUQBayesCalibration $*$ nonDMUQInstance

  Pointer to current class instance for use in static callback functions.

Friends

- class **MUQLikelihood**
- class **MUQPrior**

Additional Inherited Members

14.166.1 Detailed Description

Dakota interface to MUQ (MIT Uncertainty Quantification) library.

This class performs Bayesian calibration using the MUQ library

14.166.2 Constructor & Destructor Documentation

14.166.2.1 NonDMUQBayesCalibration (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References NonDBayesCalibration::proposalCovarType.

14.166.3 Member Function Documentation

14.166.3.1 void calibrate ( ) [protected], [virtual]

Perform the uncertainty quantification

Implements NonDBayesCalibration.

References NonDMUQBayesCalibration::cache_chain(), NonDBayesCalibration::chainSamples, Model::continuous-_variables(), WorkdirHelper::create_directory(), NonDMUQBayesCalibration::init_point, NonDMUQBayes-Calibration::log_best(), NonDBayesCalibration::mcmcModel, NonDMUQBayesCalibration::mcmcType, NonDM-UQBayesCalibration::nonDMUQInstance, Analyzer::numContinuousVars, NonDBayesCalibration::randomSeed, and WorkdirHelper::rel_to_abs().

14.166.3.2 void print_results (std::ostream & *s,* short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from NonDBayesCalibration.

References NonDBayesCalibration::bestSamples, NonDCalibration::expData, Dakota::HALF_LOG_2PI, Experiment-Data::half_log_cov_determinant(), NonDBayesCalibration::log_prior_density(), Model::num_primary_fns(), Non-DBayesCalibration::numHyperparams, NonDBayesCalibration::obsErrorMultiplierMode, NonDBayesCalibration-::print_results(), NonDMUQBayesCalibration::print_variables(), NonDBayesCalibration::residualModel, and Dakota-::write_precision.

14.166.3.3 void cache_chain ( ) [protected]

cache the chain to acceptanceChain and acceptedFnVals

Populate all of acceptanceChain(num_params, chainSamples) acceptedFnVals(numFunctions, chainSamples)

References Dakota::abort_handler(), NonDBayesCalibration::acceptanceChain, NonDBayesCalibration::accepted-FnVals, Response::active_set(), Model::active_variables(), NonDBayesCalibration::chainSamples, Variables-::continuous_variables(), Response::copy(), Variables::copy(), Model::current_response(), Model::current_-variables(), Dakota::data_pairs, Model::evaluate(), Response::function_values(), Model::interface_id(), Dakota-::lookup_by_val(), NonDBayesCalibration::mcmcModel, NonDBayesCalibration::mcmcModelHasSurrogate, Model-::model_type(), NonDMUQBayesCalibration::nonDMUQInstance, Analyzer::numContinuousVars, Analyzer::num-Functions, NonDBayesCalibration::numHyperparams, Iterator::outputLevel, Model::probability_transformation(), ActiveSet::request_values(), NonDBayesCalibration::standardizedSpace, and ParamResponsePair::variables().

Referenced by NonDMUQBayesCalibration::calibrate().

14.166.3.4 void prior_proposal_covariance ( ) [protected]

use covariance of prior distribution for setting proposal covariance

Must be called after paramMins/paramMaxs set above

References NonDBayesCalibration::mcmcModel, Model::multivariate_distribution(), Analyzer::numContinuousVars, Iterator::outputLevel, NonDMUQBayesCalibration::priorPropCovMult, NonDMUQBayesCalibration::proposalCovMatrix, and NonDBayesCalibration::standardizedSpace.

Referenced by NonDMUQBayesCalibration::init_proposal_covariance().

14.166.3.5 void user_proposal_covariance (const String & *input_fmt*, const RealVector & *cov_data*, const String & *cov_filename*) [protected]

set proposal covariance from user-provided diagonal or matrix

This function will convert user-specified cov_type = "diagonal" | "matrix" data from either cov_data or cov_filename and populate a full Eigen::MatrixXd in proposalCovMatrix with the covariance.

References Dakota::length(), Analyzer::numContinuousVars, NonDMUQBayesCalibration::proposalCovMatrix, Dakota::read_unsized_data(), and NonDBayesCalibration::standardizedSpace.

Referenced by NonDMUQBayesCalibration::init_proposal_covariance().

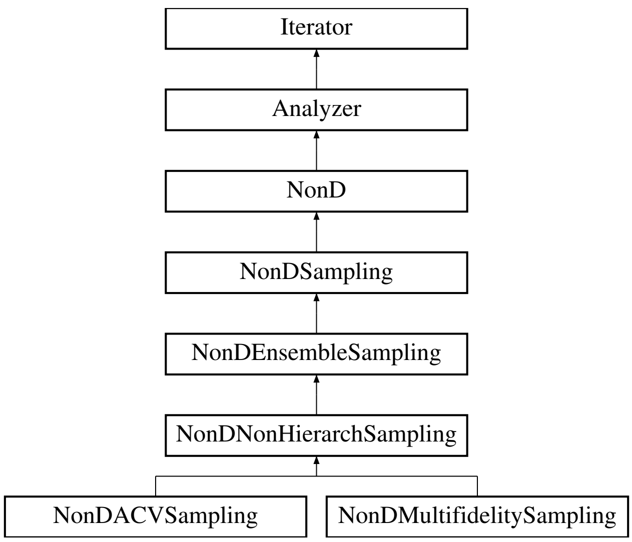
The documentation for this class was generated from the following files:

- NonDMUQBayesCalibration.hpp
- NonDMUQBayesCalibration.cpp

14.167 NonDNonHierarchSampling Class Reference

Perform Approximate Control Variate Monte Carlo sampling for UQ.

Inheritance diagram for NonDNonHierarchSampling:



Public Member Functions

- NonDNonHierarchSampling (ProblemDescDB &problem_db, Model &model)

    standard constructor

- ∼NonDNonHierarchSampling ()

  destructor

Protected Member Functions

- void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void **print_variance_reduction** (std::ostream &s)
- unsigned short uses_method () const

  return name of active optimizer method
- void method_recourse ()

  perform a numerical solver method switch due to a detected conflict
- void **shared_increment** (size_t iter)
- void **shared_approx_increment** (size_t iter)
- bool **approx_increment** (size_t iter, const SizetArray &approx_sequence, size_t start, size_t end)
- void **ensemble_sample_increment** (size_t iter, size_t step)
- void **assign_active_key** (bool multilev)
- void recover_online_cost (RealVector &seq_cost)

  recover estimates of simulation cost using aggregated response metadata
- void **initialize_sums** (IntRealMatrixMap &sum_L_baseline, IntRealVectorMap &sum_H, IntRealMatrixMap &sum_LH, RealVector &sum_HH)
- void **initialize_counts** (Sizet2DArray &num_L_baseline, SizetArray &num_H, Sizet2DArray &num_LH)
- void **finalize_counts** (Sizet2DArray &N_L)
- void **increment_equivalent_cost** (size_t new_samp, const RealVector &cost, size_t index)
- void **increment_equivalent_cost** (size_t new_samp, const RealVector &cost, size_t start, size_t end)
- void **increment_equivalent_cost** (size_t new_samp, const RealVector &cost, const SizetArray &approx_-sequence, size_t start, size_t end)
- void **compute_variance** (Real sum_Q, Real sum_QQ, size_t num_Q, Real &var_Q)
- void **compute_variance** (const RealVector &sum_Q, const RealVector &sum_QQ, const SizetArray &num_-Q, RealVector &var_Q)
- void **compute_correlation** (Real sum_Q1, Real sum_Q2, Real sum_Q1Q1, Real sum_Q1Q2, Real sum_-Q2Q2, size_t N_shared, Real &var_Q1, Real &var_Q2, Real &rho2_Q1Q2)
- void **compute_covariance** (Real sum_Q1, Real sum_Q2, Real sum_Q1Q2, size_t N_shared, Real &cov_-Q1Q2)
- void **mfmc_estvar_ratios** (const RealMatrix &rho2_LH, const SizetArray &approx_sequence, const Real-Matrix &eval_ratios, RealVector &estvar_ratios)
- void **mfmc_estvar_ratios** (const RealMatrix &rho2_LH, const SizetArray &approx_sequence, const Real-Vector &avg_eval_ratios, RealVector &estvar_ratios)
- void **mfmc_analytic_solution** (const RealMatrix &rho2_LH, const RealVector &cost, RealMatrix &eval_-ratios, bool monotonic_r=false)
- void **mfmc_reordered_analytic_solution** (const RealMatrix &rho2_LH, const RealVector &cost, SizetArray &approx_sequence, RealMatrix &eval_ratios, bool monotonic_r)
- void **cvmc_ensemble_solutions** (const RealMatrix &rho2_LH, const RealVector &cost, RealMatrix &eval_-ratios)
- void **nonhierarch_numerical_solution** (const RealVector &cost, const SizetArray &approx_sequence, Real-Vector &avg_eval_ratios, Real &avg_hf_target, size_t &num_samples, Real &avg_estvar, Real &avg_estvar-_ratio)
- Real **allocate_budget** (const RealVector &avg_eval_ratios, const RealVector &cost)
- void **scale_to_budget_with_pilot** (RealVector &avg_eval_ratios, const RealVector &cost, Real avg_N_H)
- bool ordered_approx_sequence (const RealVector &metric, SizetArray &approx_sequence, bool descending-_keys=false)

  define approx_sequence in increasing metric order
- bool ordered_approx_sequence (const RealMatrix &metric)

determine whether metric is in increasing order for all columns

- void **apply_control** (Real sum_L_shared, size_t num_shared, Real sum_L_refined, size_t num_refined, Real beta, Real &H_raw_mom)
- void inflate (const SizetArray &N_1D, Sizet2DArray &N_2D)

  promote 1D array to 2D array
- void inflate (const RealVector &avg_eval_ratios, RealMatrix &eval_ratios)

  promote vector of averaged values to full matrix
- void inflate (Real r_i, size_t num_rows, Real *eval_ratios_col)

  promote scalar to column vector
- void **compute_F_matrix** (const RealVector &avg_eval_ratios, RealSymMatrix &F)
- void **invert_CF** (const RealSymMatrix &C, const RealSymMatrix &F, RealSymMatrix &CF_inv)
- void **compute_A_vector** (const RealSymMatrix &F, const RealMatrix &c, size_t qoi, RealVector &A)
- void **compute_A_vector** (const RealSymMatrix &F, const RealMatrix &c, size_t qoi, Real var_H_q, RealVector &A)
- void **compute_Rsq** (const RealSymMatrix &CF_inv, const RealVector &A, Real var_H_q, Real &R_sq_q)
- void **acv_estvar_ratios** (const RealSymMatrix &F, RealVector &estvar_ratios)

Protected Attributes

- Iterator varianceMinimizer

  the minimizer used to minimize the estimator variance over parameters of number of truth model samples and approximation eval_ratios
- unsigned short mlmfSubMethod

  variance minimization algorithm selection: SUBMETHOD_MFMC or SUBMETHOD_ACV_{IS,MF,KL}
- size_t numApprox

  number of approximation models managed by non-hierarchical iteratedModel
- short optSubProblemForm

  formulation for optimization sub-problem that minimizes R^2 subject to different variable sets and different linear/nonlinear constraints
- unsigned short optSubProblemSolver

  SQP or NIP.
- bool truthFixedByPilot

  user specification to suppress any increments in the number of HF evaluations (e.g., because too expensive and no more can be performed)
- SizetArray approxSequence

  tracks ordering of a metric (correlations, eval ratios) across set of approximations
- SizetArray numH

  number of evaluations of HF truth model (length numFunctions)
- RealMatrix covLH

  covariances between each LF approximation and HF truth (the c vector in ACV); organized numFunctions x numApprox
- RealSymMatrixArray covLL

  covariances among all LF approximations (the C matrix in ACV); organized as a numFunctions array of symmetic numApprox x numApprox matrices
- RealMatrix rho2LH

  squared Pearson correlations among approximations and truth
- SizetArray numHIter0

  number of successful pilot evaluations of HF truth model (exclude faults)
- Real avgEstVarRatio

  ratio of final estimator variance (optimizer result averaged across QoI) and final MC estimator variance (final varH / numH averaged across QoI)

Private Member Functions

- Real objective_function (const RealVector &r_and_N)

  objective helper function shared by NPSOL/OPT++ static evaluators
- Real nonlinear_constraint (const RealVector &r_and_N)

  constraint helper function shared by NPSOL/OPT++ static evaluators
- void nonlinear_constraint_gradient (const RealVector &r_and_N, RealVector &grad_c)

  constraint gradient helper function shared by NPSOL/OPT++ static evaluators

Static Private Member Functions

- static void npsol_objective_evaluator (int &mode, int &n, double ∗x, double &f, double ∗grad_f, int &nstate)

  static function used by NPSOL for the objective function
- static void optpp_objective_evaluator (int n, const RealVector &x, double &f, int &result_mode)

  static function used by OPT++ for the objective function
- static void npsol_constraint_evaluator (int &mode, int &ncnln, int &n, int &nrowj, int ∗needc, double ∗x, double ∗c, double ∗cjac, int &nstate)

  static function used by NPSOL for the nonlinear constraints, if present
- static void optpp_constraint_evaluator (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)

  static function used by OPT++ for the nonlinear constraints, if present
- static void response_evaluator (const Variables &vars, const ActiveSet &set, Response &response)

  static function used by MinimizerAdapterModel for response data (objective and nonlinear constraint, if present)

Static Private Attributes

- static NonDNonHierarchSampling ∗ nonHierSampInstance

  pointer to NonDACV instance used in static member functions

Additional Inherited Members

14.167.1 Detailed Description

Perform Approximate Control Variate Monte Carlo sampling for UQ.

Approximate Control Variate (ACV) is a variance-reduction technique that utilitizes lower fidelity simulations that have response QoI that are correlated with the high-fidelity response QoI.

14.167.2 Constructor & Destructor Documentation

14.167.2.1 NonDNonHierarchSampling (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification. on online cost recovery through response metadata

References Dakota::abort_handler(), NonDEnsembleSampling::aggregated_models_mode(), NonD::configure_-sequence(), NonDEnsembleSampling::costMetadataIndices, ProblemDescDB::get_sza(), ProblemDescDB::get_-ushort(), Iterator::iteratedModel, NonD::load_pilot_sample(), Iterator::maxEvalConcurrency, Model::multifidelity-_precedence(), NonDEnsembleSampling::NLev, NonDNonHierarchSampling::numApprox, NonDEnsemble-Sampling::numSteps, NonDEnsembleSampling::onlineCost, NonDNonHierarchSampling::optSubProblemSolver, NonDEnsembleSampling::pilotSamples, Iterator::probDescDB, NonD::query_cost(), NonDEnsembleSampling::secondaryIndex, NonDEnsembleSampling::sequenceCost, NonDEnsembleSampling::sequenceType, NonD::sub_optimizer_select(), Model::subordinate_models(), and Model::surrogate_type().

14.167.3 Member Function Documentation

14.167.3.1 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from NonDEnsembleSampling.

References NonDNonHierarchSampling::nonHierSampInstance, NonDEnsembleSampling::pre_run(), and NonDEnsembleSampling::sequenceType.

14.167.3.2 void optpp_objective_evaluator (int *n*, const RealVector & *x*, double & *f*, int & *result_mode*) [static], [private]

static function used by OPT++ for the objective function

API for FDNLF1 objective (see SNLLOptimizer::nlf0_evaluator())

References NonDNonHierarchSampling::nonHierSampInstance, and NonDNonHierarchSampling::objective_function().

14.167.3.3 void optpp_constraint_evaluator (int *mode*, int *n*, const RealVector & *x*, RealVector & *c*, RealMatrix & *grad_c*, int & *result_mode*) [static], [private]

static function used by OPT++ for the nonlinear constraints, if present

API for NLF1 constraint (see SNLLOptimizer::constraint1_evaluator())

References NonDNonHierarchSampling::nonHierSampInstance, NonDNonHierarchSampling::nonlinear_constraint(), and NonDNonHierarchSampling::nonlinear_constraint_gradient().

14.167.3.4 void response_evaluator (const Variables & *vars*, const ActiveSet & *set*, Response & *response*) [static], [private]

static function used by MinimizerAdapterModel for response data (objective and nonlinear constraint, if present)

API for MinimizerAdapterModel

References Dakota::abort_handler(), Variables::continuous_variables(), Response::function_gradient_view(), Response::function_value(), NonDNonHierarchSampling::nonHierSampInstance, NonDNonHierarchSampling::nonlinear_constraint(), NonDNonHierarchSampling::nonlinear_constraint_gradient(), NonDNonHierarchSampling::objective_function(), and ActiveSet::request_vector().

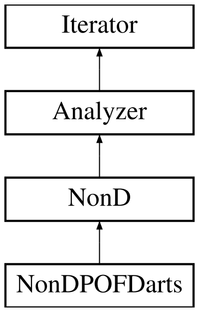
The documentation for this class was generated from the following files:

- NonDNonHierarchSampling.hpp
- NonDNonHierarchSampling.cpp

14.168 NonDPOFDarts Class Reference

Base class for POF Dart methods within DAKOTA/UQ.

Inheritance diagram for NonDPOFDarts:



Public Member Functions

- NonDPOFDarts (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDPOFDarts ()

  destructor
- bool resize ()

  reinitializes iterator based on new variable size
- void core_run ()

  perform POFDart analysis and return probability of failure

Protected Member Functions

- void initiate_random_number_generator (unsigned long x)

  POF Darts Methods.
- double **generate_a_random_number** ()
- void **init_pof_darts** ()
- void **exit_pof_darts** ()
- void **execute** (size_t kd)
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final statistics
- void **classical_dart_throwing_games** (size_t game_index)
- void **line_dart_throwing_games** (size_t game_index)
- bool **valid_dart** (double ∗x)
- bool **valid_line_flat** (size_t flat_dim, double ∗flat_dart)
- void **add_point** (double ∗x)
- void **compute_response** (double ∗x)
- void **verify_neighbor_consistency** ()
- bool **add_neighbor** (size_t ipoint, size_t ineighbor)
- void **retrieve_neighbors** (size_t ipoint, bool update_point_neighbors)
- void **sample_furthest_vertex** (size_t ipoint, double ∗fv)
- void **update_global_L** ()
- void **assign_sphere_radius_POF** (size_t isample)
- void **shrink_big_spheres** ()
- double **area_triangle** (double x1, double y1, double x2, double y2, double x3, double y3)
- void **initialize_surrogates** ()

- void **add_surrogate_data** (const Variables &vars, const Response &resp)
- void **build_surrogate** ()
- double **eval_surrogate** (size_t fn_index, double ∗vin)
- void **estimate_pof_surrogate** ()
- bool **trim_line_using_Hyperplane** (size_t num_dim, double ∗st, double ∗end, double ∗qH, double ∗nH)
- double **f_true** (double ∗x)
- void **plot_vertices_2d** (bool plot_true_function, bool plot_suurogate)
- void **plot_neighbors** ()

Protected Attributes

- int **samples**
- int **seed**
- int **emulatorSamples**
- String **lipschitzType**
- RealRealPairArray **extremeValues**
- double **Q** [1220]
- int **indx**
- double **cc**
- double **c**
- double **zc**
- double **zx**
- double **zy**
- size_t **qlen**
- bool **_eval_error**
- size_t **_test_function**
- size_t **_n_dim**
- double ∗ **_xmin**
- double ∗ **_xmax**
- double **_diag**
- double **_failure_threshold**
- double **_num_darts**
- double **_num_successive_misses_p**
- double **_num_successive_misses_m**
- double **_max_num_successive_misses**
- double **_accepted_void_ratio**
- size_t **_num_inserted_points**
- size_t **_total_budget**
- double ∗∗ **_sample_points**
- size_t ∗∗ **_sample_neighbors**
- double ∗ **_sample_vsize**
- double **_max_vsize**
- double ∗ **_dart**
- size_t **_flat_dim**
- size_t ∗ **_line_flat**
- size_t **_num_flat_segments**
- double ∗ **_line_flat_start**
- double ∗ **_line_flat_end**
- double ∗ **_line_flat_length**
- double **_safety_factor**
- double ∗ **_Lip**
- double ∗∗ **_fval**
- size_t **_active_response_function**
- bool **_use_local_L**

Additional Inherited Members

14.168.1 Detailed Description

Base class for POF Dart methods within DAKOTA/UQ.

The NonDPOFDart class implements the calculation of a failure probability for a specified threshold for a specified response function using the concepts developed by Mohamed Ebeida. The approach works by throwing down a number of Poisson disk samples of varying radii, and identifying each disk as either in the failure or safe region. The center of each disk represents a "true" function evaluation. kd-darts are used to place additional points, in such a way to target the failure region. When the disks cover the space sufficiently, Monte Carlo methods or a box volume approach is used to calculate both the lower and upper bounds on the failure probability.

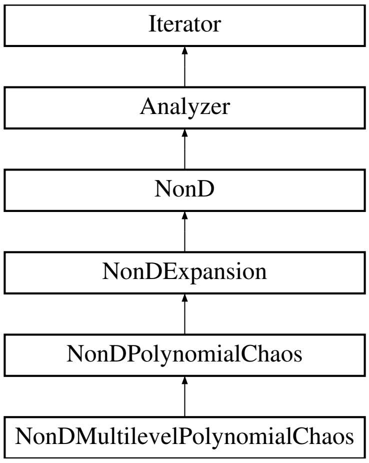
The documentation for this class was generated from the following files:

- NonDPOFDarts.hpp
- NonDPOFDarts.cpp

14.169 NonDPolynomialChaos Class Reference

Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.

Inheritance diagram for NonDPolynomialChaos:



Public Member Functions

- NonDPolynomialChaos (ProblemDescDB &problem_db, Model &model)

  standard constructor
- NonDPolynomialChaos (Model &model, short exp_coeffs_approach, unsigned short num_int, const RealVector &dim_pref, short u_space_type, short refine_type, short refine_control, short covar_control, short rule_nest, short rule_growth, bool piecewise_basis, bool use_derivs)

  alternate constructor for numerical integration (tensor, sparse, cubature)
- NonDPolynomialChaos (Model &model, short exp_coeffs_approach, unsigned short exp_order, const RealVector &dim_pref, size_t colloc_pts, Real colloc_ratio, int seed, short u_space_type, short refine_type, short refine_control, short covar_control, bool piecewise_basis, bool use_derivs, bool cv_flag, const String &import_build_pts_file, unsigned short import_build_format, bool import_build_active_only)

  alternate constructor for regression (least squares, CS, OLI)
- ∼NonDPolynomialChaos ()

  destructor

- bool resize ()

    reinitializes iterator based on new variable size

Protected Member Functions

- NonDPolynomialChaos (unsigned short method_name, ProblemDescDB &problem_db, Model &model)

    base constructor for DB construction of multilevel/multifidelity PCE (method_name is not necessary, rather it is just a convenient overload allowing the derived ML PCE class to bypass the standard PCE ctor)
- NonDPolynomialChaos (unsigned short method_name, Model &model, short exp_coeffs_approach, const RealVector &dim_pref, short u_space_type, short refine_type, short refine_control, short covar_control, short ml_alloc_control, short ml_discrep, short rule_nest, short rule_growth, bool piecewise_basis, bool use_-derivs)

    base constructor for lightweight construction of multifidelity PCE using numerical integration
- NonDPolynomialChaos (unsigned short method_name, Model &model, short exp_coeffs_approach, const RealVector &dim_pref, short u_space_type, short refine_type, short refine_control, short covar_control, const SizetArray &colloc_pts_seq, Real colloc_ratio, short ml_alloc_control, short ml_discrep, bool piecewise_-basis, bool use_derivs, bool cv_flag)

    base constructor for lightweight construction of multilevel PCE using regression
- void derived_init_communicators (ParLevLIter pl_iter)

    derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

    derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

    derived class contributions to freeing the communicators associated with this Iterator instance
- void resolve_inputs (short &u_space_type, short &data_order)

    perform error checks and mode overrides
- void initialize_u_space_model ()

    initialize uSpaceModel polynomial approximations with PCE/SC data
- size_t collocation_points () const

    return specification for number of collocation points (may be part of a sequence specification)
- void compute_expansion ()

    form the expansion by calling uSpaceModel.build_approximation()
- void select_refinement_points (const RealVectorArray &candidate_samples, unsigned short batch_size, RealMatrix &best_samples)

    evaluate allSamples for inclusion in the (PCE regression) approximation and retain the best set (well spaced) of size batch_size
- void **select_refinement_points_deprecated** (const RealVectorArray &candidate_samples, unsigned short batch_size, RealMatrix &best_samples)
- void append_expansion (const RealMatrix &samples, const IntResponseMap &resp_map)

    append new data to uSpaceModel and, when appropriate, update expansion order
- void update_samples_from_order_increment ()

    update numSamplesOnModel after an order increment
- void sample_allocation_metric (Real &sparsity_metric, Real power)

    accumulate one of the level metrics for {RIP,RANK}_SAMPLING cases
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

    print the final coefficients and final statistics
- void print_coefficients (std::ostream &s)

    print the PCE coefficient array for the orthogonal basis
- void export_coefficients ()

    export the PCE coefficient array to expansionExportFile
- void archive_coefficients ()

    archive the PCE coefficient array for the orthogonal basis

- bool config_integration (unsigned short quad_order, unsigned short ssg_level, unsigned short cub_int, Iterator &u_space_sampler, Model &g_u_model, String &approx_type)

    configure u_space_sampler and approx_type based on numerical integration specification
- bool config_expectation (size_t exp_samples, unsigned short sample_type, int seed, const String &rng, Iterator &u_space_sampler, Model &g_u_model, String &approx_type)

    configure u_space_sampler and approx_type based on expansion_samples specification
- bool config_regression (const UShortArray &exp_orders, size_t colloc_pts, Real colloc_ratio_order, short regress_type, short ls_regress_type, const UShortArray &tensor_grid_order, unsigned short sample_type, int seed, const String &rng, const String &pt_reuse, Iterator &u_space_sampler, Model &g_u_model, String &approx_type)

    configure u_space_sampler and approx_type based on regression specification
- void increment_order_from_grid ()

    define an expansion order that is consistent with an advancement in structured/unstructured grid level/density
- void ratio_samples_to_order (Real colloc_ratio, int num_samples, UShortArray &exp_order, bool less_than_or_equal)

    convert collocation ratio and number of samples to expansion order

Protected Attributes

- short uSpaceType

    user requested expansion type
- unsigned short cubIntSpec

    cubature integrand
- bool crossValidation

    flag for use of cross-validation for selection of parameter settings in regression approaches
- bool crossValidNoiseOnly

    flag to restrict cross-validation to only estimate the noise tolerance in order to manage computational cost
- unsigned short maxCVOrderCandidates

    maximum number of expansion order candidates for cross-validation in regression-based PCE
- bool respScaling

    flag for scaling response data to [0,1] for alignment with regression tols
- String importBuildPointsFile

    user-specified file for importing build points
- String expansionImportFile

    filename for import of chaos coefficients
- String expansionExportFile

    filename for export of chaos coefficients

Private Member Functions

- void order_to_dim_preference (const UShortArray &order, unsigned short &p, RealVector &dim_pref)

    convert an isotropic/anisotropic expansion_order vector into a scalar plus a dimension preference vector

Private Attributes

- RealVector noiseTols

    noise tolerance for compressive sensing algorithms; vector form used in cross-validation
- Real l2Penalty

    L2 penalty for LASSO algorithm (elastic net variant)
- unsigned short numAdvance

    number of frontier expansions per iteration with the ADAPTED_BASIS_EXPANDING_FRONT approach

- unsigned short expOrderSpec

  user specification for expansion_order (array for multifidelity)
- size_t collocPtsSpec

  user specification for collocation_points (array for multifidelity)
- size_t expSamplesSpec

  user specification for expansion_samples (array for multifidelity)
- unsigned short quadOrderSpec

  user request of quadrature order
- unsigned short ssgLevelSpec

  user request of sparse grid level
- RealMatrix pceGradsMeanX

  derivative of the PCE with respect to the x-space variables evaluated at the means (used as uncertainty importance metrics)
- bool normalizedCoeffOutput

  user request for use of normalization when outputting PCE coefficients

Additional Inherited Members

14.169.1 Detailed Description

Nonintrusive polynomial chaos expansion approaches to uncertainty quantification.

The NonDPolynomialChaos class uses a polynomial chaos expansion (PCE) approach to approximate the effect of parameter uncertainties on response functions of interest. It utilizes the OrthogPolyApproximation class to manage multiple types of orthogonal polynomials within a Wiener-Askey scheme to PCE. It supports PCE coefficient estimation via sampling, quadrature, point-collocation, and file import.

14.169.2 Constructor & Destructor Documentation

14.169.2.1 NonDPolynomialChaos (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation using the ProblemDescDB.

References Dakota::abort_handler(), Model::assign_rep(), NonDPolynomialChaos::collocPtsSpec, ParallelLibrary::command_line_check(), NonDPolynomialChaos::config_expectation(), NonDPolynomialChaos::config_integration(), NonDPolynomialChaos::config_regression(), NonDExpansion::configure_expansion_orders(), NonDExpansion::construct_expansion_sampler(), NonDPolynomialChaos::cubIntSpec, ActiveSet::derivative_vector(), NonDExpansion::dimPrefSpec, NonDPolynomialChaos::expansionImportFile, NonDPolynomialChaos::expOrderSpec, NonDPolynomialChaos::expSamplesSpec, ProblemDescDB::get_bool(), ProblemDescDB::get_iv(), ProblemDescDB::get_real(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), ProblemDescDB::get_usa(), ProblemDescDB::get_ushort(), NonDPolynomialChaos::importBuildPointsFile, NonDPolynomialChaos::initialize_u_space_model(), Iterator::iteratedModel, NonDExpansion::numSamplesOnModel, Iterator::outputLevel, Iterator::parallelLib, NonDPolynomialChaos::quadOrderSpec, NonDExpansion::randomSeed, NonDPolynomialChaos::resolve_inputs(), NonDPolynomialChaos::ssgLevelSpec, NonDExpansion::uSpaceModel, and NonDPolynomialChaos::uSpaceType.

14.169.2.2 NonDPolynomialChaos (Model & *model,* short *exp_coeffs_approach,* unsigned short *num_int,* const RealVector & *dim_pref,* short *u_space_type,* short *refine_type,* short *refine_control,* short *covar_control,* short *rule_nest,* short *rule_growth,* bool *piecewise_basis,* bool *use_derivs*)

alternate constructor for numerical integration (tensor, sparse, cubature)

This constructor is used for helper iterator instantiation on the fly that employ numerical integration (quadrature, sparse grid, cubature).

References Dakota::abort_handler(), Response::active_set(), Model::assign_rep(), NonDPolynomialChaos::config_integration(), Model::current_response(), ActiveSet::derivative_vector(), NonDPolynomialChaos::initialize_u_space_model(), Iterator::iteratedModel, Iterator::outputLevel, Model::qoi(), NonDPolynomialChaos::resolve_inputs(), NonDExpansion::uSpaceModel, and NonDPolynomialChaos::uSpaceType.

14.169.2.3 NonDPolynomialChaos (Model & *model*, short *exp_coeffs_approach*, unsigned short *exp_order*, const RealVector & *dim_pref*, size_t *colloc_pts*, Real *colloc_ratio*, int *seed*, short *u_space_type*, short *refine_type*, short *refine_control*, short *covar_control*, bool *piecewise_basis*, bool *use_derivs*, bool *cv_flag*, const String & *import_build_pts_file*, unsigned short *import_build_format*, bool *import_build_active_only*)

alternate constructor for regression (least squares, CS, OLI)

This constructor is used for helper iterator instantiation on the fly that employ regression (least squares, CS, OLI).

References Response::active_set(), Model::assign_rep(), NonDPolynomialChaos::collocPtsSpec, NonDPolynomialChaos::config_regression(), NonDExpansion::configure_expansion_orders(), Model::current_response(), ActiveSet::derivative_vector(), NonDExpansion::dimPrefSpec, NonDPolynomialChaos::expOrderSpec, NonDPolynomialChaos::importBuildPointsFile, NonDPolynomialChaos::initialize_u_space_model(), Iterator::iteratedModel, Iterator::outputLevel, Model::qoi(), NonDExpansion::randomSeed, NonDPolynomialChaos::resolve_inputs(), NonDExpansion::uSpaceModel, and NonDPolynomialChaos::uSpaceType.

14.169.2.4 NonDPolynomialChaos (unsigned short *method_name*, ProblemDescDB & *problem_db*, Model & *model*) [protected]

base constructor for DB construction of multilevel/multifidelity PCE (method_name is not necessary, rather it is just a convenient overload allowing the derived ML PCE class to bypass the standard PCE ctor)

This constructor is called by derived class constructors that customize the object construction.

14.169.2.5 NonDPolynomialChaos (unsigned short *method_name*, Model & *model*, short *exp_coeffs_approach*, const RealVector & *dim_pref*, short *u_space_type*, short *refine_type*, short *refine_control*, short *covar_control*, short *ml_alloc_control*, short *ml_discrep*, short *rule_nest*, short *rule_growth*, bool *piecewise_basis*, bool *use_derivs*) [protected]

base constructor for lightweight construction of multifidelity PCE using numerical integration

This constructor is called by derived class constructors for lightweight instantiations that employ numerical integration (quadrature, sparse grid, cubature).

References NonDExpansion::multilevAllocControl, and NonDExpansion::multilevDiscrepEmulation.

14.169.2.6 NonDPolynomialChaos (unsigned short *method_name*, Model & *model*, short *exp_coeffs_approach*, const RealVector & *dim_pref*, short *u_space_type*, short *refine_type*, short *refine_control*, short *covar_control*, const SizetArray & *colloc_pts_seq*, Real *colloc_ratio*, short *ml_alloc_control*, short *ml_discrep*, bool *piecewise_basis*, bool *use_derivs*, bool *cv_flag*) [protected]

base constructor for lightweight construction of multilevel PCE using regression

This constructor is called by derived class constructors for lightweight instantiations that employ regression (least squares, CS, OLI).

References NonDExpansion::collocPtsSeqSpec, NonDExpansion::multilevAllocControl, and NonDExpansion::multilevDiscrepEmulation.

14.169.3 Member Function Documentation

14.169.3.1 void increment_order_from_grid ( ) [protected]

define an expansion order that is consistent with an advancement in structured/unstructured grid level/density

Used for uniform refinement of regression-based PCE.

References NonDExpansion::collocRatio, SharedApproxData::data_rep(), SharedPecosApproxData::expansion_order(), NonDExpansion::numSamplesOnModel, NonDPolynomialChaos::ratio_samples_to_order(), Model::shared_approximation(), and NonDExpansion::uSpaceModel.

Referenced by NonDPolynomialChaos::append_expansion().

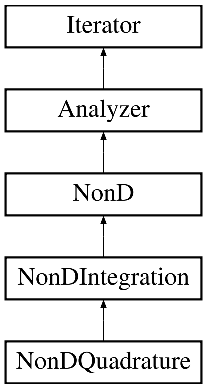
The documentation for this class was generated from the following files:

- NonDPolynomialChaos.hpp
- NonDPolynomialChaos.cpp

14.170 NonDQuadrature Class Reference

Derived nondeterministic class that generates N-dimensional numerical quadrature points for evaluation of expectation integrals over uncorrelated standard normals/uniforms/exponentials/betas/gammas.

Inheritance diagram for NonDQuadrature:



Public Member Functions

- NonDQuadrature (Model &model, unsigned short quad_order, const RealVector &dim_pref, short driver_mode)

  alternate constructor for instantiations "on the fly" based on a quadrature order specification
- NonDQuadrature (Model &model, unsigned short quad_order, const RealVector &dim_pref, short driver_mode, int num_filt_samples)

  alternate constructor for instantiations "on the fly" that filter a tensor product sample set to include points with highest sample weights
- NonDQuadrature (Model &model, unsigned short quad_order, const RealVector &dim_pref, short driver_mode, int num_sub_samples, int seed)

  alternate constructor for instantiations "on the fly" that sub-sample quadrature rules by sampling randomly from a tensor product multi-index
- ∼NonDQuadrature ()

  destructor
- void increment_grid ()

  increment SSG level/TPQ order
- void decrement_grid ()

  decrement SSG level/TPQ order

- void evaluate_grid_increment ()

    computes a grid increment and evaluates the new parameter sets
- void update ()

    propagate any numSamples updates and/or grid updates/increments
- void reset ()

    set Pecos::TensorProductDriver::quadOrder to dimension orders indicated by quadOrderSpec & dimPrefSpec, following refinement or sequence advancement
- const Pecos::UShortArray & quadrature_order () const

    return Pecos::TensorProductDriver::quadOrder
- void quadrature_order (const Pecos::UShortArray &dim_quad_order)

    set Pecos::TensorProductDriver::quadOrder
- void quadrature_order (unsigned short quad_order)

    set quadOrderSpec and map to Pecos::TensorProductDriver::quadOrder
- void samples (size_t samples)

    set numSamples
- short mode () const

    return quadMode

Protected Member Functions

- NonDQuadrature (ProblemDescDB &problem_db, Model &model)

    constructor
- void initialize_grid (const std::vector< Pecos::BasisPolynomial > &poly_basis)
- void get_parameter_sets (Model &model)

    Generate one block of numSamples samples (ndim $*$ num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.
- void sampling_reset (size_t min_samples, bool all_data_flag, bool stats_flag)
- void sampling_reference (size_t samples_ref)

    set reference number of samples, which is a lower bound during reset
- void increment_grid_preference (const RealVector &dim_pref)

    increment SSG level/TPQ order and update anisotropy
- void increment_grid_preference ()

    increment SSG level/TPQ order and preserve anisotropy
- size_t num_samples () const
- void random_seed (int seed)

    set randomSeed, if present

Private Member Functions

- void increment_grid (UShortArray &ref_quad_order)

    convenience function used to make increment_grid() more modular
- void increment_grid_preference (const RealVector &dim_pref, UShortArray &ref_quad_order)

    convenience function used to make increment_grid_preference() more modular
- void decrement_grid (UShortArray &ref_quad_order)

    convenience function used to make decrement_grid() more modular
- void compute_minimum_quadrature_order (size_t min_samples, const RealVector &dim_pref)

    calculate smallest dimension quadrature order with at least min_samples and propagate to Pecos::TensorProductDriver
- void filter_parameter_sets ()

    prune allSamples back to size numSamples, retaining points with highest product weight
- void update_anisotropic_order (const RealVector &dim_pref, UShortArray &quad_order_ref)

update quad_order_ref based on an updated dimension preference, enforcing previous values as a lower bound

- void initialize_dimension_quadrature_order (unsigned short quad_order_spec, const RealVector &dim_pref_spec)

  initialize Pecos::TensorProductDriver::quadOrder from quad_order_spec and dim_pref_spec
- void increment_reference_quadrature_order (UShortArray &ref_quad_order)

  increment each ref_quad_order entry by 1
- void increment_reference_quadrature_order (const RealVector &dim_pref, UShortArray &ref_quad_order)

  increment the ref_quad_order entry with maximum preference by 1 and then rebalance

Private Attributes

- std::shared_ptr
  < Pecos::TensorProductDriver > tpqDriver

  convenience pointer to the numIntDriver representation
- bool nestedRules

  for studies involving refinement strategies, allow for use of nested quadrature rules such as Gauss-Patterson
- unsigned short quadOrderSpec

  scalar quadrature order, rendered anisotropic via dimPrefSpec
- UShortArray refQuadOrderPrev

  value of Pecos::TensorProductDriver::quadOrder prior to increment_grid(), for restoration in decrement_grid() (increment must induce a change in grid size and this increment may not be reversible). Since this data is not keyed, increment/decrement must occur together prior to a key change.
- short quadMode

  point generation mode: FULL_TENSOR, FILTERED_TENSOR, RANDOM_TENSOR
- size_t numSamples

  size of a subset of tensor quadrature points (filtered based on product weight or sampled uniformly from the tensor multi-index); used by the regression PCE approach known as "probabilistic collocation"
- int randomSeed

  seed for the random number generator used in sampling of the tensor multi-index

Additional Inherited Members

14.170.1 Detailed Description

Derived nondeterministic class that generates N-dimensional numerical quadrature points for evaluation of expectation integrals over uncorrelated standard normals/uniforms/exponentials/betas/gammas.

This class is used by NonDPolynomialChaos, but could also be used for general numerical integration of moments. It employs Gauss-Hermite, Gauss-Legendre, Gauss-Laguerre, Gauss-Jacobi and generalized Gauss--Laguerre quadrature for use with normal, uniform, exponential, beta, and gamma density functions and integration bounds. The abscissas and weights for one-dimensional integration are extracted from the appropriate OrthogonalPolynomial class and are extended to n-dimensions using a tensor product approach.

14.170.2 Constructor & Destructor Documentation

14.170.2.1 NonDQuadrature (Model & *model,* unsigned short *quad_order,* const RealVector & *dim_pref,* short *driver_mode*)

alternate constructor for instantiations "on the fly" based on a quadrature order specification

This alternate constructor is used for on-the-fly generation and evaluation of numerical quadrature points.

References NonDIntegration::numIntDriver, and NonDQuadrature::tpqDriver.

14.170.2.2 NonDQuadrature (Model & *model*, unsigned short *quad_order*, const RealVector & *dim_pref*, short *driver_mode*, int *num_filt_samples*)

alternate constructor for instantiations "on the fly" that filter a tensor product sample set to include points with highest sample weights

This alternate constructor is used for on-the-fly generation and evaluation of filtered tensor quadrature points.

References NonDIntegration::numIntDriver, and NonDQuadrature::tpqDriver.

14.170.2.3 NonDQuadrature (Model & *model*, unsigned short *quad_order*, const RealVector & *dim_pref*, short *driver_mode*, int *num_sub_samples*, int *seed*)

alternate constructor for instantiations "on the fly" that sub-sample quadrature rules by sampling randomly from a tensor product multi-index

This alternate constructor is used for on-the-fly generation and evaluation of random sampling from a tensor quadrature multi-index.

References NonDIntegration::numIntDriver, and NonDQuadrature::tpqDriver.

14.170.2.4 NonDQuadrature (ProblemDescDB & *problem_db*, Model & *model*) [protected]

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification. It is not currently used, as there is not yet a separate nond_quadrature method specification.

References Iterator::convergenceTol, Model::correction_type(), ProblemDescDB::get_bool(), ProblemDescDB::get_short(), ProblemDescDB::get_sizet(), ProblemDescDB::get_ushort(), Iterator::iteratedModel, Iterator::maxEvalConcurrency, Model::multivariate_distribution(), NonDQuadrature::nestedRules, NonDIntegration::numIntDriver, Iterator::outputLevel, Iterator::probDescDB, NonDQuadrature::reset(), and NonDQuadrature::tpqDriver.

14.170.3 Member Function Documentation

14.170.3.1 void initialize_grid (const std::vector< Pecos::BasisPolynomial > & *poly_basis*) [protected], [virtual]

Used in combination with alternate NonDQuadrature constructor.

Implements NonDIntegration.

References Iterator::iteratedModel, Iterator::maxEvalConcurrency, Model::multivariate_distribution(), NonDQuadrature::nestedRules, Analyzer::numContinuousVars, NonDQuadrature::numSamples, NonDQuadrature::quadMode, NonDQuadrature::reset(), NonDQuadrature::tpqDriver, and NonDQuadrature::update().

14.170.3.2 void sampling_reset (size_t *min_samples*, bool *all_data_flag*, bool *stats_flag*) [protected], [virtual]

used by DataFitSurrModel::build_global() to publish the minimum number of points needed from the quadrature routine in order to build a particular global approximation.

Reimplemented from Iterator.

References NonDIntegration::dimPrefSpec, NonDQuadrature::increment_grid(), NonDQuadrature::increment_grid_preference(), NonDQuadrature::numSamples, and NonDQuadrature::tpqDriver.

Referenced by NonDQuadrature::update().

14.170.3.3 size_t num_samples ( ) const [inline], [protected], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.

References NonDQuadrature::numSamples, NonDQuadrature::quadMode, and NonDQuadrature::tpqDriver.

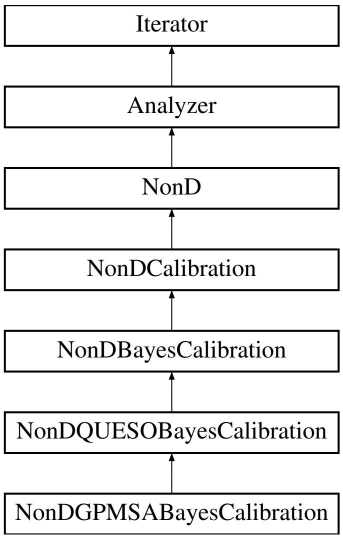
The documentation for this class was generated from the following files:

- NonDQuadrature.hpp
- NonDQuadrature.cpp

14.171 NonDQUESOBayesCalibration Class Reference

Bayesian inference using the QUESO library from UT Austin.

Inheritance diagram for NonDQUESOBayesCalibration:



Public Member Functions

- NonDQUESOBayesCalibration (ProblemDescDB &problem_db, Model &model)

  standard constructor
- ∼NonDQUESOBayesCalibration ()

  destructor

Protected Member Functions

- void calibrate ()
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS) override

  print the final iterator results
- void init_queso_environment ()

  initialize the QUESO FullEnvironment on the Dakota MPIComm
- void init_precond_request_value ()

  initialize the ASV value for preconditioned cases
- void specify_prior () override

intialize the QUESO parameter space, min, max, initial, domain, and prior define solver options, likelihood callback, posterior RV, and inverse problem

- void **specify_likelihood** () override
- void **init_bayesian_solver** () override
- void **specify_posterior** () override
- void precondition_proposal (unsigned int chain_index)

  use derivative information from the emulator to define the proposal covariance (inverse of misfit Hessian)
- void run_queso_solver ()

  perform the MCMC process
- void **map_pre_solve** () override
- void run_chain ()

  short term option to restart the MCMC chain with updated proposal density computed from the emulator at a new starting point
- void cache_chain ()

  cache the chain to acceptanceChain and acceptedFnVals
- void log_best ()

  log at most batchSize best chain points into bestSamples
- void filter_chain_by_conditioning () override

  extract batchSize points from the MCMC chain and store final aggregated set within allSamples; unique points with best conditioning are selected, as determined by pivoted LU
- void **init_proposal_covariance** ()
- void prior_proposal_covariance ()

  use covariance of prior distribution for setting proposal covariance
- void user_proposal_covariance (const String &input_fmt, const RealVector &cov_data, const String &cov_-filename)

  Set proposal covariance from user-provided diagonal or matrix.
- void **validate_proposal** ()
- void set_ip_options ()

  Set inverse problem options calIpOptionsValues common to all solvers.
- void set_mh_options ()

  Set MH-specific inverse problem options calIpMhOptionsValues.
- void update_chain_size (unsigned int size)

  update MH-specific inverse problem options calIpMhOptionsValues
- void copy_gsl (const QUESO::GslVector &qv, RealVector &rv)

  local copy_data utility from GslVector to RealVector
- void copy_gsl (const RealVector &rv, QUESO::GslVector &qv)

  local copy_data utility from RealVector to GslVector
- void copy_gsl_partial (const QUESO::GslVector &qv, size_t start, RealVector &rv)

  local copy_data utility from portion of GslVector to RealVector
- void copy_gsl_partial (const RealVector &rv, QUESO::GslVector &qv, size_t start)

  local copy_data utility from RealVector to portion of GslVector
- void copy_gsl (const QUESO::GslVector &qv, RealMatrix &rm, int i)

  local copy_data utility from GslVector to column in RealMatrix
- bool equal_gsl (const QUESO::GslVector &qv1, const QUESO::GslVector &qv2)

  equality tester for two GslVectors

Static Protected Member Functions

- static double dakotaLogLikelihood (const QUESO::GslVector &paramValues, const QUESO::GslVector ∗paramDirection, const void ∗functionDataPtr, QUESO::GslVector ∗gradVector, QUESO::GslMatrix ∗hessian-Matrix, QUESO::GslVector ∗hessianEffect)

  Log Likelihood function for call-back from QUESO to DAKOTA for evaluation.

Protected Attributes

- String mcmcType

  MCMC type ("dram" or "delayed_rejection" or "adaptive_metropolis" or "metropolis_hastings" or "multilevel", within QUESO)
- int propCovUpdatePeriod

  period (number of accepted chain samples) for proposal covariance update
- short precondRequestValue

  the active set request value to use in proposal preconditioning
- bool logitTransform

  flag indicating user activation of logit transform option
- std::shared_ptr
  < QUESO::EnvOptionsValues > envOptionsValues

  options for setting up the QUESO Environment
- std::shared_ptr
  < QUESO::FullEnvironment > quesoEnv

  top-level QUESO Environment
- std::shared_ptr
  < QUESO::VectorSpace
  < QUESO::GslVector,
  QUESO::GslMatrix > > paramSpace

  QUESO parameter space based on number of calibrated parameters.
- std::shared_ptr
  < QUESO::BoxSubset
  < QUESO::GslVector,
  QUESO::GslMatrix > > paramDomain

  QUESO parameter domain: hypercube based on min/max values.
- std::shared_ptr< QUESO::GslVector > paramInitials

  initial parameter values at which to start chain
- std::shared_ptr
  < QUESO::BaseVectorRV
  < QUESO::GslVector,
  QUESO::GslMatrix > > priorRv

  random variable for the prior
- std::shared_ptr< QUESO::GslMatrix > proposalCovMatrix

  proposal covariance for DRAM
- double priorPropCovMult

  optional multiplier to scale prior-based proposal covariance
- std::shared_ptr
  < QUESO::SipOptionsValues > calIpOptionsValues

  general inverse problem options
- std::shared_ptr
  < QUESO::MhOptionsValues > calIpMhOptionsValues

  MH-specific inverse problem options.
- std::shared_ptr
  < QUESO::GenericScalarFunction
  < QUESO::GslVector,
  QUESO::GslMatrix > > **likelihoodFunctionObj**
- std::shared_ptr
  < QUESO::GenericVectorRV
  < QUESO::GslVector,
  QUESO::GslMatrix > > postRv

  random variable for the posterior

- std::shared_ptr
< QUESO::StatisticalInverseProblem
< QUESO::GslVector,
QUESO::GslMatrix > > inverseProb

    QUESO inverse problem solver.
- String advancedOptionsFile

    advanced options file name (GPMSA only); settings from this file override any C++ / Dakota input file settings

Static Protected Attributes

- static NonDQUESOBayesCalibration ∗ nonDQUESOInstance

    Pointer to current class instance for use in static callback functions.

Friends

- class DerivInformedPropCovTK< QUESO::GslVector, QUESO::GslMatrix >

    Random walk transition kernel needs callback access to QUESO details.
- class DerivInformedPropCovLogitTK< QUESO::GslVector, QUESO::GslMatrix >

    Logit random walk transition kernel needs callback access to QUESO details.

Additional Inherited Members

14.171.1 Detailed Description

Bayesian inference using the QUESO library from UT Austin.

This class wraps the Quantification of Uncertainty for Estimation, Simulation, and Optimization (QUESO) library, developed as part of the Predictive Science Academic Alliance Program (PSAAP)-funded Predictive Engineering and Computational Sciences (PECOS) Center at UT Austin.

14.171.2 Constructor & Destructor Documentation

14.171.2.1 NonDQUESOBayesCalibration (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDQUESOBayesCalibration::advancedOptionsFile, NonDCalibration::calibrationData, NonDBayesCalibration::chainSamples, NonDBayesCalibration::emulatorType, NonDQUESOBayesCalibration::init_queso_environment(), NonDBayesCalibration::obsErrorMultiplierMode, Iterator::outputLevel, NonDQUESOBayesCalibration::priorPropCovMult, NonDQUESOBayesCalibration::propCovUpdatePeriod, and NonDBayesCalibration::proposalCovarType.

14.171.3 Member Function Documentation

14.171.3.1 void calibrate ( ) [protected], [virtual]

Perform the uncertainty quantification

Implements NonDBayesCalibration.

References NonDQUESOBayesCalibration::run_chain().

14.171.3.2 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [override], [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from NonDBayesCalibration.

References NonDBayesCalibration::bestSamples, NonDQUESOBayesCalibration::copy_gsl(), NonDQUESOBayesCalibration::copy_gsl_partial(), NonDCalibration::expData, Dakota::HALF_LOG_2PI, ExperimentData::half_log_cov_determinant(), NonDBayesCalibration::log_prior_density(), Model::num_primary_fns(), Analyzer::numContinuousVars, NonDBayesCalibration::obsErrorMultiplierMode, NonDQUESOBayesCalibration::paramSpace, NonDBayesCalibration::print_results(), NonDBayesCalibration::print_variables(), NonDBayesCalibration::residualModel, and Dakota::write_precision.

14.171.3.3 void specify_prior ( ) [override], [protected], [virtual]

intialize the QUESO parameter space, min, max, initial, domain, and prior define solver options, likelihood callback, posterior RV, and inverse problem

Initialize the calibration parameter domain (paramSpace, paramMins/paramMaxs, paramDomain, paramInitials, priorRV)

Reimplemented from NonDBayesCalibration.

References NonDQUESOBayesCalibration::copy_gsl(), NonDBayesCalibration::mapSoln, NonDBayesCalibration::mcmcModel, Model::multivariate_distribution(), NonDQUESOBayesCalibration::nonDQUESOInstance, Analyzer::numContinuousVars, NonDBayesCalibration::numHyperparams, Iterator::outputLevel, NonDQUESOBayesCalibration::paramDomain, NonDQUESOBayesCalibration::paramInitials, NonDQUESOBayesCalibration::paramSpace, NonDQUESOBayesCalibration::priorRv, and NonDQUESOBayesCalibration::quesoEnv.

14.171.3.4 void cache_chain ( ) [protected]

cache the chain to acceptanceChain and acceptedFnVals

Populate all of acceptanceChain(num_params, chainSamples) acceptedFnVals(numFunctions, chainSamples)

References Dakota::abort_handler(), NonDBayesCalibration::acceptanceChain, NonDBayesCalibration::acceptedFnVals, Response::active_set(), Model::active_variables(), NonDBayesCalibration::chainSamples, Variables::continuous_variables(), Response::copy(), Variables::copy(), NonDQUESOBayesCalibration::copy_gsl_partial(), Model::current_response(), Model::current_variables(), Dakota::data_pairs, Model::evaluate(), Response::function_values(), Model::interface_id(), Dakota::lookup_by_val(), NonDBayesCalibration::mcmcModel, NonDBayesCalibration::mcmcModelHasSurrogate, Model::model_type(), Analyzer::numContinuousVars, Analyzer::numFunctions, NonDBayesCalibration::numHyperparams, Iterator::outputLevel, NonDQUESOBayesCalibration::postRv, Model::probability_transformation(), ActiveSet::request_values(), NonDBayesCalibration::standardizedSpace, and ParamResponsePair::variables().

Referenced by NonDQUESOBayesCalibration::run_chain().

14.171.3.5 void prior_proposal_covariance ( ) [protected]

use covariance of prior distribution for setting proposal covariance

Must be called after paramMins/paramMaxs set above

References NonDBayesCalibration::mcmcModel, Model::multivariate_distribution(), Analyzer::numContinuousVars, Iterator::outputLevel, NonDQUESOBayesCalibration::priorPropCovMult, NonDQUESOBayesCalibration::proposalCovMatrix, and NonDBayesCalibration::standardizedSpace.

14.171.3.6 void user_proposal_covariance (const String & *input_fmt*, const RealVector & *cov_data*, const String & *cov_filename*) [protected]

Set proposal covariance from user-provided diagonal or matrix.

This function will convert user-specified cov_type = "diagonal" | "matrix" data from either cov_data or cov_filename and populate a full QUESO::GslMatrix∗ in proposalCovMatrix with the covariance.

References Dakota::length(), Analyzer::numContinuousVars, NonDQUESOBayesCalibration::proposalCovMatrix, Dakota::read_unsized_data(), and NonDBayesCalibration::standardizedSpace.

14.171.3.7 void set_ip_options ( ) [protected]

Set inverse problem options calIpOptionsValues common to all solvers.

set inverse problem options common to all solvers

References NonDQUESOBayesCalibration::advancedOptionsFile, NonDQUESOBayesCalibration::calIpOptionsValues, Iterator::outputLevel, and NonDQUESOBayesCalibration::quesoEnv.

Referenced by NonDGPMSABayesCalibration::init_queso_solver().

14.171.4 Member Data Documentation

14.171.4.1 bool logitTransform [protected]

flag indicating user activation of logit transform option

this option is useful for preventing rejection or resampling for out-of-bounds samples by transforming bounded domains to [-inf,inf].

Referenced by NonDQUESOBayesCalibration::set_mh_options().

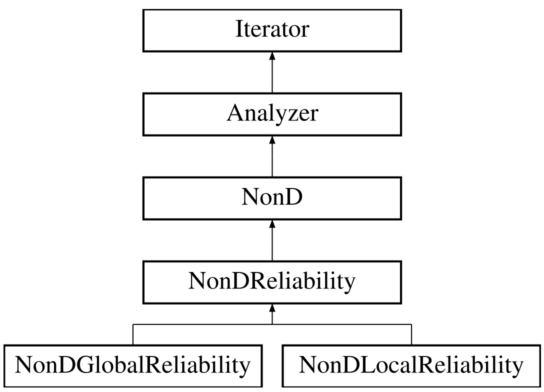
The documentation for this class was generated from the following files:

- NonDQUESOBayesCalibration.hpp
- NonDQUESOBayesCalibration.cpp

14.172 NonDReliability Class Reference

Base class for the reliability methods within DAKOTA/UQ.

Inheritance diagram for NonDReliability:



Protected Member Functions

- NonDReliability (ProblemDescDB &problem_db, Model &model)

    constructor
- ∼NonDReliability ()

    destructor
- void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

    set primaryA{CV,DIV,DRV}MapIndices, secondaryA{CV,DIV,DRV}MapTargets within derived Iterators; supports computation of higher-level sensitivities in nested contexts (e.g., derivatives of statistics w.r.t. inserted design variables)
- bool resize ()

    reinitializes iterator based on new variable size
- void post_run (std::ostream &s)

    post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- const Model & algorithm_space_model () const

Protected Attributes

- Model uSpaceModel

    Model representing the limit state in u-space, after any recastings and data fits.
- Model mppModel

    RecastModel which formulates the optimization subproblem: RIA, PMA, EGO.
- Iterator mppOptimizer

    Iterator which optimizes the mppModel.
- unsigned short mppSearchType

    the MPP search type selection: Local: MV, x/u-space {AMV,AMV+,TANA,QMEA} or NO_APPROX Global x/u-space EGRA
- Iterator importanceSampler

    importance sampling instance used to compute/refine probabilities
- unsigned short integrationRefinement

    integration refinement type (NO_INT_REFINE, IS, AIS, or MMAIS) provided by `refinement` *specification*
- size_t numRelAnalyses

    number of invocations of core_run()
- size_t approxIters

    number of approximation cycles for the current respFnCount/levelCount
- bool approxConverged

    indicates convergence of approximation-based iterations
- int respFnCount

    counter for which response function is being analyzed
- size_t levelCount

    counter for which response/probability level is being analyzed
- size_t statCount

    counter for which final statistic is being computed
- bool pmaMaximizeG

    flag indicating maximization of G(u) within PMA formulation
- Real requestedTargetLevel

    the {response,reliability,generalized reliability} level target for the current response function

Additional Inherited Members

14.172.1 Detailed Description

Base class for the reliability methods within DAKOTA/UQ.

The NonDReliability class provides a base class for NonDLocalReliability, which implements traditional MPP-based reliability methods, and NonDGlobalReliability, which implements global limit state search using Gaussian process models in combination with multimodal importance sampling.

14.172.2 Member Function Documentation

14.172.2.1 void post_run (std::ostream & *s*) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Analyzer.

References Model::finalize_mapping(), Model::is_null(), NonDReliability::mppModel, NonDReliability::numRel-Analyses, and Analyzer::post_run().

14.172.2.2 const Model & algorithm_space_model ( ) const [inline], [protected], [virtual]

default definition that gets redefined in selected derived Minimizers

Reimplemented from Analyzer.

References NonDReliability::uSpaceModel.

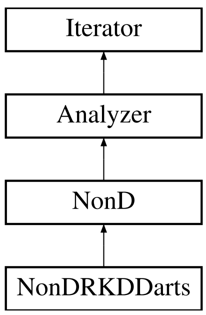
The documentation for this class was generated from the following files:

- NonDReliability.hpp
- NonDReliability.cpp

14.173 NonDRKDDarts Class Reference

Base class for the Recursive k-d Dart methods within DAKOTA/UQ.

Inheritance diagram for NonDRKDDarts:



Public Member Functions

- NonDRKDDarts (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼NonDRKDDarts ()

  destructor
- bool resize ()

  reinitializes iterator based on new variable size
- void core_run ()

Protected Member Functions

- void pre_run ()

  generate samples
- void **initiate_random_number_generator** (unsigned long x)
- double **generate_a_random_number** ()
- void **init_rkd_darts** ()
- void **create_rkd_containers** (size_t expected_num_samples)
- void **execute** ()
- void **create_initial_children** (size_t parent)
- void **create_new_sample** (size_t parent, size_t left, size_t right, double position)
- void **improve_parent_evaluation** (size_t parent)
- void **evaluate_1d_surrogate** (size_t parent)
- double **get_surrogate_interp_error** (size_t parent)
- double **estimate_surrogate_evaluation_err** (size_t parent)
- void **get_children** (size_t parent, size_t ∗children)
- void **get_neighbors** (size_t sample, size_t &num_neighbors, size_t ∗neighbors)
- double **interpolate_lagrange** (size_t num_data_points, double ∗data_x, double ∗data_f, double x)
- double **integrate_legendre_gauss** (double xmin, double xmax, size_t num_data_points, double ∗data_x, double ∗data_f, double &err_est)
- double **f_true** (double ∗x)
- void **initialize_surrogates** ()
- void **compute_response** (double ∗x)
- void **add_surrogate_data** (const Variables &vars, const Response &resp)
- void **build_surrogate** ()
- double **eval_surrogate** (size_t fn_index, double ∗vin)
- void **estimate_rkd_surrogate** ()
- void post_run (std::ostream &s)

- void **print_integration_results** (std::ostream &s)
- void **exit_rkd_darts** ()
- void **destroy_rkd_containers** ()

Protected Attributes

- int **samples**
- int **seed**
- int **emulatorSamples**
- double **Q** [1220]
- int **indx**
- double **cc**
- double **c**
- double **zc**
- double **zx**
- double **zy**
- size_t **qlen**

Private Attributes

- double ∗ **_I_RKD**
- bool **_eval_error**
- size_t **_test_function**
- size_t **_num_inserted_points**
- size_t **_num_dim**
- size_t **_num_samples**
- size_t **_max_num_samples**
- size_t **_num_evaluations**
- size_t **_evaluation_budget**
- size_t **_max_num_neighbors**
- double **_bounding_box_volume**
- double **_discont_jump_threshold**
- double ∗ **_xmin**
- double ∗ **_xmax**
- double ∗∗ **_fval**
- size_t ∗ **_sample_dim**
- size_t ∗ **_sample_parent**
- size_t ∗ **_sample_first_child**
- size_t ∗ **_sample_num_children**
- size_t ∗ **_sample_left**
- size_t ∗ **_sample_right**
- double ∗ **_sample_coord**
- double ∗ **_sample_value**
- double ∗ **_sample_left_interp_err**
- double ∗ **_sample_right_interp_err**
- double ∗ **_sample_left_ev_err**
- double ∗ **_sample_right_ev_err**

Additional Inherited Members

14.173.1 Detailed Description

Base class for the Recursive k-d Dart methods within DAKOTA/UQ.

The NonDRKDDart class recursively implements the numerical integration of a domain based on k-d flat samples.

14.173.2 Member Function Documentation

14.173.2.1 void core_run ( ) [virtual]

Loop over the set of samples and compute responses.

Reimplemented from Iterator.

14.173.2.2 void pre_run ( ) [protected], [virtual]

generate samples

Generate Parameter Sets.

Reimplemented from Analyzer.

References Analyzer::pre_run().

14.173.2.3 void post_run (std::ostream & s) [protected], [virtual]

generate statistics

Print function evaluation summary, and integration results.

Reimplemented from Analyzer.

References Iterator::iteratedModel, Analyzer::post_run(), and Model::print_evaluation_summary().

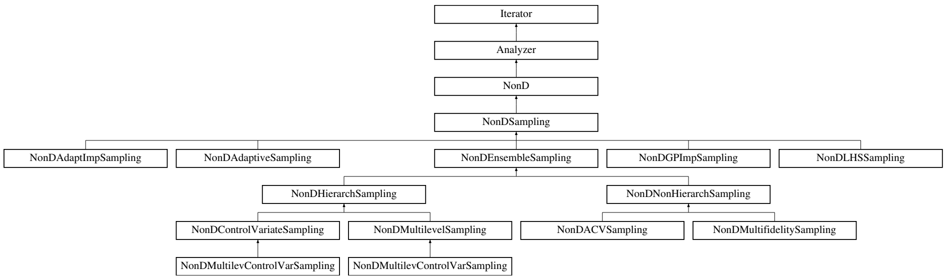
The documentation for this class was generated from the following files:

- NonDRKDDarts.hpp
- NonDRKDDarts.cpp

14.174 NonDSampling Class Reference

Base class for common code between NonDLHSSampling, NonDAdaptImpSampling, and other specializations.

Inheritance diagram for NonDSampling:



Public Member Functions

- NonDSampling (Model &model, const RealMatrix &sample_matrix)

    alternate constructor for evaluating and computing statistics for the provided set of samples
- ∼NonDSampling ()

    destructor
- void compute_statistics (const RealMatrix &vars_samples, const IntResponseMap &resp_samples)

    For the input sample set, computes mean, standard deviation, and probability/reliability/response levels (aleatory uncertainties) or intervals (epsitemic or mixed uncertainties)
- void compute_intervals (RealRealPairArray &extreme_fns)

    called by compute_statistics() to calculate min/max intervals using allResponses
- void compute_intervals (const IntResponseMap &samples)

    called by compute_statistics() to calculate extremeValues from samples
- void compute_intervals (RealRealPairArray &extreme_fns, const IntResponseMap &samples)

    called by compute_statistics() to calculate min/max intervals using samples
- void compute_moments (const RealVectorArray &fn_samples)

    calculates sample moments from a matrix of observations for a set of QoI
- void compute_moments (const IntResponseMap &samples)

    calculate sample moments and confidence intervals from a map of response observations
- void compute_moments (const IntResponseMap &samples, RealMatrix &moment_stats, RealMatrix &moment_grads, RealMatrix &moment_conf_ints, short moments_type, const StringArray &labels)

    convert IntResponseMap to RealVectorArray and invoke helpers
- void compute_moment_gradients (const RealVectorArray &fn_samples, const RealMatrixArray &grad_-samples, const RealMatrix &moment_stats, RealMatrix &moment_grads, short moments_type)

compute moment_grads from function and gradient samples

- void compute_moment_confidence_intervals (const RealMatrix &moment_stats, RealMatrix &moment_conf-_ints, const SizetArray &sample_counts, short moments_type)

  compute moment confidence intervals from moment values
- void archive_moments (size_t inc_id=0)

  archive moment statistics in results DB
- void archive_moment_confidence_intervals (size_t inc_id=0)

  archive moment confidence intervals in results DB
- void archive_extreme_responses (size_t inc_id=0)

  archive extreme values (epistemic result) in results DB
- void compute_level_mappings (const IntResponseMap &samples)

  called by compute_statistics() to calculate CDF/CCDF mappings of z to p/beta and of p/beta to z as well as PDFs
- void print_statistics (std::ostream &s) const

  prints the statistics computed in compute_statistics()
- void print_intervals (std::ostream &s) const

  prints the intervals computed in compute_intervals() with default qoi_type and moment_labels
- void print_intervals (std::ostream &s, String qoi_type, const StringArray &interval_labels) const

  prints the intervals computed in compute_intervals()
- void print_moments (std::ostream &s) const

  prints the moments computed in compute_moments() with default qoi_type and moment_labels
- void print_moments (std::ostream &s, String qoi_type, const StringArray &moment_labels) const

  prints the moments computed in compute_moments()
- void print_wilks_stastics (std::ostream &s) const

  prints the Wilks stastics
- void update_final_statistics ()

  update finalStatistics from minValues/maxValues, momentStats, and computedProbLevels/computedRel-Levels/computedRespLevels
- void transform_samples (Pecos::ProbabilityTransformation &nataf, bool x_to_u=true)

  transform allSamples imported by alternate constructor. This is needed since random variable distribution parameters are not updated until run time and an imported sample_matrix is typically in x-space.
- void transform_samples (Pecos::ProbabilityTransformation &nataf, RealMatrix &sample_matrix, size_t num_-samples=0, bool x_to_u=true)

  transform the specified samples matrix from x to u or u to x
- unsigned short sampling_scheme () const

  return sampleType
- const String & random_number_generator () const

  return rngName

Static Public Member Functions

- static void compute_moments (const RealVectorArray &fn_samples, SizetArray &sample_counts, RealMatrix &moment_stats, short moments_type, const StringArray &labels)

  core compute_moments() implementation with all data as inputs
- static void compute_moments (const RealVectorArray &fn_samples, RealMatrix &moment_stats, short moments_type)

  core compute_moments() implementation with all data as inputs
- static void compute_moments (const RealMatrix &fn_samples, RealMatrix &moment_stats, short moments-_type)

  alternate RealMatrix samples API for use by external clients
- static void print_moments (std::ostream &s, const RealMatrix &moment_stats, const RealMatrix moment_cis, String qoi_type, short moments_type, const StringArray &moment_labels, bool print_cis)

  core print moments that can be called without object

- static int compute_wilks_sample_size (unsigned short order, Real alpha, Real beta, bool twosided=false)

    calculates the number of samples using the Wilks formula Static so I can test without instantiating a NonDSampling object - RWH
- static Real compute_wilks_residual (unsigned short order, int nsamples, Real alpha, Real beta, bool twosided)

    Helper function - calculates the Wilks residual.
- static Real compute_wilks_alpha (unsigned short order, int nsamples, Real beta, bool twosided=false)

    calculates the alpha paramter given number of samples using the Wilks formula Static so I can test without instantiating a NonDSampling object - RWH
- static Real compute_wilks_beta (unsigned short order, int nsamples, Real alpha, bool twosided=false)

    calculates the beta paramter given number of samples using the Wilks formula Static so I can test without instantiating a NonDSampling object - RWH
- static Real get_wilks_alpha_min ()

    Get the lower and upper bounds supported by Wilks bisection solves.
- static Real **get_wilks_alpha_max** ()
- static Real **get_wilks_beta_min** ()
- static Real **get_wilks_beta_max** ()

Protected Member Functions

- NonDSampling (ProblemDescDB &problem_db, Model &model)

    constructor
- NonDSampling (unsigned short method_name, Model &model, unsigned short sample_type, size_t samples, int seed, const String &rng, bool vary_pattern, short sampling_vars_mode)

    alternate constructor for sample generation and evaluation "on the fly"
- NonDSampling (unsigned short sample_type, size_t samples, int seed, const String &rng, const RealVector &lower_bnds, const RealVector &upper_bnds)

    alternate constructor for sample generation "on the fly"
- NonDSampling (unsigned short sample_type, size_t samples, int seed, const String &rng, const RealVector &means, const RealVector &std_devs, const RealVector &lower_bnds, const RealVector &upper_bnds, RealSymMatrix &correl)

    alternate constructor for sample generation of correlated normals "on the fly"
- void pre_run ()

    pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()
- size_t num_samples () const
- void sampling_reset (size_t min_samples, bool all_data_flag, bool stats_flag)

    resets number of samples and sampling flags
- void sampling_reference (size_t samples_ref)

    set reference number of samples, which is a lower bound during reset
- void random_seed (int seed)

    assign randomSeed
- void vary_pattern (bool pattern_flag)

    set varyPattern
- void get_parameter_sets (Model &model)

    Uses lhsDriver to generate a set of samples from the distributions/bounds defined in the incoming model.
- void get_parameter_sets (Model &model, const size_t num_samples, RealMatrix &design_matrix)

    Uses lhsDriver to generate a set of samples from the distributions/bounds defined in the incoming model and populates the specified design matrix.
- void get_parameter_sets (Model &model, const size_t num_samples, RealMatrix &design_matrix, bool write_msg)

core of get_parameter_sets that accepts message print control

- void get_parameter_sets (const RealVector &lower_bnds, const RealVector &upper_bnds)

  Uses lhsDriver to generate a set of uniform samples over lower_bnds/upper_bnds.
- void get_parameter_sets (const RealVector &means, const RealVector &std_devs, const RealVector &lower-_bnds, const RealVector &upper_bnds, RealSymMatrix &correl)

  Uses lhsDriver to generate a set of normal samples.
- void update_model_from_sample (Model &model, const Real *sample_vars)

  Override default update of continuous vars only.
- void sample_to_variables (const Real *sample_vars, Variables &vars)

  override default mapping of continuous variables only
- void variables_to_sample (const Variables &vars, Real *sample_vars)

  override default mapping of continuous variables only
- const RealSymMatrix & response_error_estimates () const

  return error estimates associated with each of the finalStatistics
- virtual bool seed_updated ()

  detect whether the seed has been updated since the most recent sample set generation
- virtual void active_set_mapping ()

  in the case of sub-iteration, map from finalStatistics.active_set() requests to activeSet used in evaluate_parameter_-sets()
- void initialize_sample_driver (bool write_message, size_t num_samples)

  increments numLHSRuns, sets random seed, and initializes lhsDriver
- void mode_counts (const Variables &vars, size_t &cv_start, size_t &num_cv, size_t &div_start, size_t &num-_div, size_t &dsv_start, size_t &num_dsv, size_t &drv_start, size_t &num_drv) const

  compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model
- void mode_bits (const Variables &vars, BitArray &active_vars, BitArray &active_corr) const

  define subset views for sampling modes

Protected Attributes

- int seedSpec

  the user seed specification (default is 0)
- int randomSeed

  the current seed
- const int samplesSpec

  initial specification of number of samples
- size_t samplesRef

  reference number of samples updated for refinement
- size_t numSamples

  the current number of samples to evaluate
- String rngName

  name of the random number generator
- unsigned short sampleType

  `the sample type: default, random, lhs,`
  < incremental random, or incremental lhs
- bool wilksFlag

  flags use of Wilks formula to calculate num samples
- unsigned short **wilksOrder**
- Real **wilksAlpha**
- Real **wilksBeta**
- short **wilksSidedness**
- RealMatrix momentGrads

gradients of standardized or central moments of response functions, as determined by finalMomentsType. Calculated in compute_moments() and indexed as (var,moment) when moment id runs from 1:2∗numFunctions.

- RealSymMatrix finalStatErrors

  standard errors (estimator std deviation) for each of the finalStatistics
- int samplesIncrement

  current increment in a sequence of samples
- Pecos::LHSDriver lhsDriver

  the C++ wrapper for the F90 LHS library
- size_t numLHSRuns

  counter for number of sample set generations
- bool statsFlag

  flags computation/output of statistics
- bool allDataFlag

  `flags update of allResponses`
  < (allVariables or allSamples already defined)
- short samplingVarsMode

  the sampling mode: ALEATORY_UNCERTAIN{,_UNIFORM}, EPISTEMIC_UNCERTAIN{,_UNIFORM}, UNCERTAIN{,_UNIFORM}, ACTIVE{,_UNIFORM}, or ALL{,_UNIFORM}. This is a secondary control on top of the variables view that allows sampling over subsets of variables that may differ from the view.
- short sampleRanksMode

  mode for input/output of LHS sample ranks: IGNORE_RANKS, GET_RANKS, SET_RANKS, or SET_GET_RANKS
- bool varyPattern

  flag for generating a sequence of seed values within multiple get_parameter_sets() calls so that these executions (e.g., for SBO/SBNLS) are not repeated, but are still repeatable
- RealMatrix sampleRanks

  data structure to hold the sample ranks
- SensAnalysisGlobal nonDSampCorr

  initialize statistical post processing
- bool backfillFlag

  flags whether to use backfill to enforce uniqueness of discrete LHS samples
- RealRealPairArray extremeValues

  Minimum and maximum values of response functions for epistemic calculations (calculated in compute_intervals()),.
- bool functionMomentsComputed

  Function moments have been computed; used to determine whether to archive the moments.

Private Member Functions

- void sample_to_variables (const Real ∗sample_vars, Variables &vars, Model &model)

  helper function to consolidate update code
- void sample_to_type (const Real ∗sample_vars, Variables &vars, size_t &cv_index, size_t num_cv, size_t &div_index, size_t num_div, size_t &dsv_index, size_t num_dsv, size_t &drv_index, size_t num_drv, size_t &samp_index, Model &model)

  helper function to copy a range from sample_vars to a variables type
- void sample_to_cv_type (const Real ∗sample_vars, Variables &vars, size_t &cv_index, size_t num_cv, size_t &div_index, size_t num_div, size_t &dsv_index, size_t num_dsv, size_t &drv_index, size_t num_drv, size_t &samp_index)

  helper function to copy a range from sample_vars to a variables type
- void sample_to_cv (const Real ∗sample_vars, Variables &vars, size_t &acv_index, size_t num_acv, size_t &samp_index)

  helper function to copy a range from sample_vars to continuous variables
- void sample_to_div (const Real ∗sample_vars, Variables &vars, size_t &adiv_index, size_t num_adiv, size_t &samp_index)

helper function to copy a range from sample_vars to discrete int variables

- void sample_to_dsv (const Real ∗sample_vars, Variables &vars, size_t &adsv_index, size_t num_adsv, size_t &samp_index, const StringSetArray &dss_values)

    helper function to copy a range from sample_vars to discrete string vars

- void sample_to_drv (const Real ∗sample_vars, Variables &vars, size_t &adrv_index, size_t num_adrv, size_t &samp_index)

    helper function to copy a range from sample_vars to discrete real vars

Private Attributes

- RealMatrix momentCIs

    Matrix of confidence internals on moments, with rows for mean_lower, mean_upper, sd_lower, sd_upper (calculated in compute_moments())

Additional Inherited Members

14.174.1 Detailed Description

Base class for common code between NonDLHSSampling, NonDAdaptImpSampling, and other specializations.

This base class provides common code for sampling methods which employ the Latin Hypercube Sampling (LHS) package from Sandia Albuquerque's Risk and Reliability organization. NonDSampling now exclusively utilizes the 1998 Fortran 90 LHS version as documented in SAND98-0210, which was converted to a UNIX link library in

1. The 1970's vintage LHS (that had been f2c'd and converted to incomplete classes) has been removed.

14.174.2 Constructor & Destructor Documentation

14.174.2.1 NonDSampling (Model & *model,* const RealMatrix & *sample_matrix*)

alternate constructor for evaluating and computing statistics for the provided set of samples

This alternate constructor defines allSamples from an incoming sample matrix.

References Analyzer::allSamples, Analyzer::compactMode, Iterator::maxEvalConcurrency, NonDSampling::numSamples, NonDSampling::samplesRef, NonDSampling::samplesSpec, and Iterator::subIteratorFlag.

14.174.2.2 NonDSampling (ProblemDescDB & *problem_db,* Model & *model*) [protected]

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

References Dakota::abort_handler(), NonDSampling::compute_wilks_sample_size(), NonD::epistemicStats, ProblemDescDB::get_real(), ProblemDescDB::get_short(), ProblemDescDB::get_ushort(), Iterator::maxEvalConcurrency, Analyzer::numFunctions, NonDSampling::numSamples, Iterator::probDescDB, NonD::requestedProbLevels, NonDSampling::samplesRef, NonDSampling::sampleType, NonD::totalLevelRequests, and NonDSampling::wilksFlag.

14.174.2.3 NonDSampling (unsigned short *method_name,* Model & *model,* unsigned short *sample_type,* size_t *samples,* int *seed,* const String & *rng,* bool *vary_pattern,* short *sampling_vars_mode*) [protected]

alternate constructor for sample generation and evaluation "on the fly"

This alternate constructor is used for generation and evaluation of on-the-fly sample sets.

References SharedVariablesData::active_components_totals(), Model::current_variables(), NonD::epistemicStats, Iterator::iteratedModel, Iterator::maxEvalConcurrency, NonDSampling::numSamples, NonDSampling::sampleType, NonDSampling::samplingVarsMode, Variables::shared_data(), and Iterator::subIteratorFlag.

14.174.2.4 NonDSampling (unsigned short *sample_type,* size_t *samples,* int *seed,* const String & *rng,* const RealVector & *lower_bnds,* const RealVector & *upper_bnds*) [protected]

alternate constructor for sample generation "on the fly"

This alternate constructor is used by ConcurrentStrategy for generation of uniform, uncorrelated sample sets.

References Iterator::maxEvalConcurrency, NonDSampling::numSamples, NonDSampling::sampleType, and Iterator::subIteratorFlag.

14.174.2.5 NonDSampling (unsigned short *sample_type,* size_t *samples,* int *seed,* const String & *rng,* const RealVector & *means,* const RealVector & *std_devs,* const RealVector & *lower_bnds,* const RealVector & *upper_bnds,* RealSymMatrix & *correl*) [protected]

alternate constructor for sample generation of correlated normals "on the fly"

This alternate constructor is used by ConcurrentStrategy for generation of normal, correlated sample sets.

References Iterator::maxEvalConcurrency, NonDSampling::numSamples, NonDSampling::sampleType, and Iterator::subIteratorFlag.

14.174.3 Member Function Documentation

14.174.3.1 void compute_level_mappings (const IntResponseMap & *samples*)

called by compute_statistics() to calculate CDF/CCDF mappings of z to p/beta and of p/beta to z as well as PDFs

Computes CDF/CCDF based on sample binning. A PDF is inferred from a CDF/CCDF within compute_densities() after level computation.

References Dakota::abort_handler(), Response::active_set_derivative_vector(), Response::active_set_request-_vector(), NonD::archive_allocate_mappings(), NonD::cdfFlag, NonD::compute_densities(), NonD::computed-GenRelLevels, NonD::computedProbLevels, NonD::computedRelLevels, NonD::computedRespLevels, NonD-Sampling::extremeValues, NonD::finalMomentsType, NonD::finalStatistics, Response::function_gradient_view(), NonD::initialize_level_mappings(), Iterator::iteratedModel, NonDSampling::momentGrads, NonD::momentStats, Analyzer::numFunctions, NonD::pdfOutput, NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD-::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, and Model::response_labels().

Referenced by NonDSampling::compute_statistics().

14.174.3.2 void transform_samples (Pecos::ProbabilityTransformation & *nataf,* bool *x_to_u* = true) [inline]

transform allSamples imported by alternate constructor. This is needed since random variable distribution parameters are not updated until run time and an imported sample_matrix is typically in x-space.

transform x_samples to u_samples for use by expansionSampler

References Analyzer::allSamples, and NonDSampling::numSamples.

Referenced by NonDLHSSampling::d_optimal_parameter_set().

14.174.3.3 void pre_run ( ) [inline], [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

References NonDSampling::active_set_mapping(), Analyzer::pre_run(), and Iterator::subIteratorFlag.

Referenced by NonDEnsembleSampling::pre_run(), and NonDLHSSampling::pre_run().

14.174.3.4 void core_run ( ) [protected], [virtual]

Default implementation generates allResponses from either allSamples or allVariables.

Reimplemented from Iterator.

References NonDSampling::allDataFlag, Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, and NonDSampling::statsFlag.

14.174.3.5 size_t num_samples ( ) const [inline], [protected], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.

References NonDSampling::numSamples.

Referenced by NonDLHSSampling::archive_results(), NonDAdaptImpSampling::evaluate_samples(), NonDSampling::get_parameter_sets(), NonDSampling::initialize_sample_driver(), NonDSampling::print_wilks_stastics(), NonDAdaptImpSampling::select_rep_points(), NonDLHSSampling::store_ranks(), and NonDSampling::transform_samples().

14.174.3.6 void sampling_reset (size_t *min_samples*, bool *all_data_flag*, bool *stats_flag*) [inline], [protected], [virtual]

resets number of samples and sampling flags

used by DataFitSurrModel::build_global() to publish the minimum number of samples needed from the sampling routine (to build a particular global approximation) and to set allDataFlag and statsFlag. In this case, allDataFlag is set to true (vectors of variable and response sets must be returned to build the global approximation) and statsFlag is set to false (statistics computations are not needed).

Reimplemented from Iterator.

References NonDSampling::allDataFlag, NonDSampling::numSamples, NonDSampling::samplesIncrement, NonDSampling::samplesRef, and NonDSampling::statsFlag.

14.174.3.7 void get_parameter_sets (Model & *model*) [inline], [protected], [virtual]

Uses lhsDriver to generate a set of samples from the distributions/bounds defined in the incoming model.

This version of get_parameter_sets() extracts data from the user-defined model in any of the four sampling modes and populates class member allSamples.

Reimplemented from Analyzer.

References Analyzer::allSamples, and NonDSampling::numSamples.

Referenced by NonDLHSSampling::compute_pca(), NonDAdaptImpSampling::core_run(), NonDLHSSampling::d_optimal_parameter_set(), NonDMultilevelSampling::evaluate_ml_sample_increment(), NonDSampling::get_parameter_sets(), NonDLHSSampling::increm_lhs_parameter_set(), NonDLHSSampling::initial_increm_lhs_set(), NonDControlVariateSampling::lf_increment(), NonDLHSSampling::NonDLHSSampling(), NonDLHSSampling::pre_run(), and NonDControlVariateSampling::shared_increment().

14.174.3.8 void get_parameter_sets (Model & *model*, const size_t *num_samples*, RealMatrix & *design_matrix*) [inline], [protected], [virtual]

Uses lhsDriver to generate a set of samples from the distributions/bounds defined in the incoming model and populates the specified design matrix.

This version of get_parameter_sets() extracts data from the user-defined model in any of the four sampling modes and populates the specified design matrix.

Reimplemented from Analyzer.

References NonDSampling::get_parameter_sets().

14.174.3.9 void get_parameter_sets (const RealVector & *lower_bnds*, const RealVector & *upper_bnds*) [protected]

Uses lhsDriver to generate a set of uniform samples over lower_bnds/upper_bnds.

This version of get_parameter_sets() does not extract data from the user-defined model, but instead relies on the incoming bounded region definition. It only support a UNIFORM sampling mode, where the distinction of ACTIVE_UNIFORM vs. ALL_UNIFORM is handled elsewhere.

References Analyzer::allSamples, NonDSampling::initialize_sample_driver(), NonDSampling::lhsDriver, and NonDSampling::numSamples.

14.174.3.10 void get_parameter_sets (const RealVector & *means*, const RealVector & *std_devs*, const RealVector & *lower_bnds*, const RealVector & *upper_bnds*, RealSymMatrix & *correl*) [protected]

Uses lhsDriver to generate a set of normal samples.

This version of get_parameter_sets() does not extract data from the user-defined model, but instead relies on the incoming definition. It only supports the sampling of normal variables.

References Analyzer::allSamples, NonDSampling::initialize_sample_driver(), NonDSampling::lhsDriver, and NonDSampling::numSamples.

14.174.3.11 void active_set_mapping ( ) [protected], [virtual]

in the case of sub-iteration, map from finalStatistics.active_set() requests to activeSet used in evaluate_parameter_sets()

Map ASV/DVV requests in final statistics into activeSet for use in evaluate_parameter_sets()

Reimplemented in NonDEnsembleSampling.

References Response::active_set_derivative_vector(), Response::active_set_request_vector(), Iterator::activeSet, ActiveSet::derivative_vector(), NonD::finalMomentsType, NonD::finalStatistics, Analyzer::numFunctions, ActiveSet::request_vector(), NonD::requestedGenRelLevels, NonD::requestedProbLevels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, and NonD::totalLevelRequests.

Referenced by NonDEnsembleSampling::active_set_mapping(), and NonDSampling::pre_run().

14.174.3.12 void mode_counts (const Variables & *vars*, size_t & *cv_start*, size_t & *num_cv*, size_t & *div_start*, size_t & *num_div*, size_t & *dsv_start*, size_t & *num_dsv*, size_t & *drv_start*, size_t & *num_drv*) const [protected]

compute sampled subsets (all, active, uncertain) within all variables (acv/adiv/adrv) from samplingVarsMode and model

This function and its helpers to follow are needed since NonDSampling supports a richer set of sampling modes than just the active variable subset. mode_counts() manages the samplingVarsMode setting, while its helper functions (view_{design,aleatory_uncertain,epistemic_uncertain, uncertain,state}_counts) manage the active variables view. Similar to the computation of starts and counts in creating active variable views, the results of this function are starts and counts for use within model.all_∗() set/get functions.

References Variables::acv(), Variables::adiv(), Variables::adrv(), Variables::adsv(), SharedVariablesData::aleatory-_uncertain_counts(), Variables::cv(), Variables::cv_start(), SharedVariablesData::design_counts(), Variables::div(), Variables::div_start(), Variables::drv(), Variables::drv_start(), Variables::dsv(), Variables::dsv_start(), Shared-VariablesData::epistemic_uncertain_counts(), NonDSampling::samplingVarsMode, Variables::shared_data(), SharedVariablesData::state_counts(), Dakota::svd(), and SharedVariablesData::uncertain_counts().

Referenced by NonDLHSSampling::archive_results(), NonDSampling::compute_statistics(), NonDLHSSampling-::d_optimal_parameter_set(), NonDSampling::get_parameter_sets(), NonDLHSSampling::post_input(), NonDLHS-Sampling::pre_run(), NonDSampling::print_statistics(), and NonDSampling::variables_to_sample().

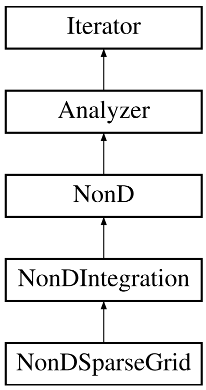
The documentation for this class was generated from the following files:

- NonDSampling.hpp
- NonDSampling.cpp

14.175 NonDSparseGrid Class Reference

Derived nondeterministic class that generates N-dimensional Smolyak sparse grids for numerical evaluation of expectation integrals over independent standard random variables.

Inheritance diagram for NonDSparseGrid:



Public Member Functions

- NonDSparseGrid (Model &model, unsigned short ssg_level, const RealVector &dim_pref, short exp_coeffs_-soln_approach, short driver_mode, short growth_rate=Pecos::MODERATE_RESTRICTED_GROWTH, short refine_control=Pecos::NO_CONTROL, bool track_uniq_prod_wts=true)
- ∼NonDSparseGrid ()

  destructor
- void sparse_grid_level (unsigned short ssg_level)

  update the sparse grid level (e.g., from a level sequence)
- void increment_grid ()

  increment ssgDriver::ssgLevel
- void increment_grid_weights (const RealVector &aniso_wts)

  update ssgDriver::ssgAnisoLevelWts and increment ssgDriver::ssgLevel based on specified anisotropic weighting
- void increment_grid_weights ()

increment ssgDriver::ssgLevel based on existing anisotropic weighting
- void decrement_grid ()

  decrement ssgDriver::ssgLevel
- void evaluate_grid_increment ()

  computes a grid increment and evaluates the new parameter sets
- void push_grid_increment ()

  restores a previously computed grid increment (no new evaluations)
- void pop_grid_increment ()

  removes a previously computed grid increment
- void merge_grid_increment ()

  merges a grid increment into the reference grid
- void reset ()

  reset ssgDriver level and dimension preference back to {ssgLevel,dimPref}Spec for the active key, following refinement or sequence advancement
- void reset_all ()

  blow away all data for all keys
- const std::set< UShortArray > & active_multi_index () const

  returns SparseGridDriver::active_multi_index()
- void print_smolyak_multi_index () const

  invokes SparseGridDriver::print_smolyak_multi_index()
- void initialize_sets ()

  invokes SparseGridDriver::initialize_sets()
- void update_reference ()

  invokes SparseGridDriver::update_reference()
- void increment_set (const UShortArray &set)

  invokes SparseGridDriver::increment_smolyak_multi_index()
- int increment_size () const

  invokes SparseGridDriver::unique_trial_points()
- void push_set ()

  invokes SparseGridDriver::push_set()
- void evaluate_set ()

  invokes SparseGridDriver::compute_trial_grid()
- void decrement_set ()

  invokes SparseGridDriver::pop_set()
- void update_sets (const UShortArray &set_star)

  invokes SparseGridDriver::update_sets()
- void finalize_sets (bool output_sets, bool converged_within_tol, bool reverted)

  invokes SparseGridDriver::finalize_sets()
- size_t num_samples () const

Protected Member Functions

- NonDSparseGrid (ProblemDescDB &problem_db, Model &model)

  constructor
- void initialize_grid (const std::vector< Pecos::BasisPolynomial > &poly_basis)

  initialize integration grid by drawing from polynomial basis settings
- void get_parameter_sets (Model &model)

  Generate one block of numSamples samples (ndim $*$ num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.
- void sampling_reset (size_t min_samples, bool all_data_flag, bool stats_flag)
- const RealVector & **anisotropic_weights** () const

Private Attributes

- short ssgDriverType

  type of sparse grid driver: combined, incremental, hierarchical, ...
- std::shared_ptr
  < Pecos::SparseGridDriver > ssgDriver

  convenience pointer to the numIntDriver representation
- unsigned short ssgLevelSpec

  the user specification for the Smolyak sparse grid level, rendered anisotropic via dimPrefSpec
- unsigned short ssgLevelPrev

  value of ssgDriver->level() prior to increment_grid(), for restoration in decrement_grid() since increment must induce a change in grid size and this adaptive increment in not reversible

Additional Inherited Members

14.175.1 Detailed Description

Derived nondeterministic class that generates N-dimensional Smolyak sparse grids for numerical evaluation of expectation integrals over independent standard random variables.

This class is used by NonDPolynomialChaos and NonDStochCollocation, but could also be used for general numerical integration of moments. It employs 1-D Clenshaw-Curtis and Gaussian quadrature rules within Smolyak sparse grids.

14.175.2 Constructor & Destructor Documentation

14.175.2.1 NonDSparseGrid (Model & *model,* unsigned short *ssg_level,* const RealVector & *dim_pref,* short *exp_coeffs_soln_approach,* short *driver_mode,* short *growth_rate* = Pecos::MODERATE_RESTRICTED_GROWTH*,* short *refine_control* = Pecos::NO_CONTROL*,* bool *track_uniq_prod_wts* = true)

This alternate constructor is used for on-the-fly generation and evaluation of sparse grids within PCE and SC.

References NonDIntegration::numIntDriver, NonDSparseGrid::ssgDriver, and NonDSparseGrid::ssgDriverType.

14.175.2.2 NonDSparseGrid (ProblemDescDB & *problem_db,* Model & *model*) [protected]

constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification. It is not currently used, as there is not a separate sparse_grid method specification.

References Iterator::convergenceTol, Model::correction_type(), NonDIntegration::dimPrefSpec, ProblemDescDB::get_bool(), ProblemDescDB::get_short(), ProblemDescDB::get_sizet(), ProblemDescDB::get_ushort(), NonDSparseGrid::initialize_grid(), Iterator::maxEvalConcurrency, Model::multivariate_distribution(), NonDIntegration::numIntDriver, Iterator::outputLevel, Iterator::probDescDB, NonDSparseGrid::ssgDriver, NonDSparseGrid::ssgDriverType, and NonDSparseGrid::ssgLevelSpec.

14.175.3 Member Function Documentation

14.175.3.1 size_t num_samples ( ) const [inline], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.

References NonDSparseGrid::ssgDriver.

14.175.3.2 void sampling_reset (size_t *min_samples*, bool *all_data_flag*, bool *stats_flag*) [protected], [virtual]

used by DataFitSurrModel::build_global() to publish the minimum number of points needed from the sparse grid routine in order to build a particular global approximation.

Reimplemented from Iterator.

References NonDSparseGrid::ssgDriver.

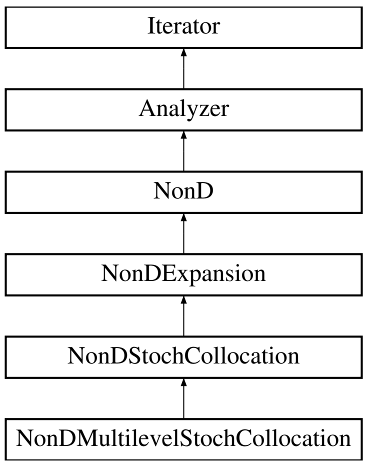
The documentation for this class was generated from the following files:

- NonDSparseGrid.hpp
- NonDSparseGrid.cpp

14.176 NonDStochCollocation Class Reference

Nonintrusive stochastic collocation approaches to uncertainty quantification.

Inheritance diagram for NonDStochCollocation:



Public Member Functions

- NonDStochCollocation (ProblemDescDB &problem_db, Model &model)

    standard constructor
- NonDStochCollocation (Model &model, short exp_coeffs_approach, unsigned short num_int, const RealVector &dim_pref, short u_space_type, short refine_type, short refine_control, short covar_control, short rule_nest, short rule_growth, bool piecewise_basis, bool use_derivs)

    alternate constructor
- ∼NonDStochCollocation ()

    destructor
- bool resize ()

    reinitializes iterator based on new variable size

Protected Member Functions

- NonDStochCollocation (unsigned short method_name, ProblemDescDB &problem_db, Model &model)

short-cut ctor allowing derived class to replace logic in base class ctor (method_name is not necessary, rather it is just a convenient overload allowing the derived ML SC class to bypass the standard SC ctor)

- NonDStochCollocation (unsigned short method_name, Model &model, short exp_coeffs_approach, const RealVector &dim_pref, short refine_type, short refine_control, short covar_control, short ml_alloc_control, short ml_discrep, short rule_nest, short rule_growth, bool piecewise_basis, bool use_derivs)

  short-cut ctor allowing derived class to replace logic in base class ctor
- void resolve_inputs (short &u_space_type, short &data_order)

  perform error checks and mode overrides
- void initialize_u_space_model ()

  initialize uSpaceModel polynomial approximations with PCE/SC data
- Real compute_covariance_metric (bool revert, bool print_metric)

  compute 2-norm of change in response covariance
- Real compute_level_mappings_metric (bool revert, bool print_metric)

  compute 2-norm of change in final statistics
- void initialize_covariance ()

  initialize covariance pairings by passing all pointers for approximation j to approximation i
- void compute_delta_mean (bool update_ref)

  helper function to compute deltaRespVariance
- void compute_delta_variance (bool update_ref, bool print_metric)

  helper function to compute deltaRespVariance
- void compute_delta_covariance (bool update_ref, bool print_metric)

  helper function to compute deltaRespCovariance
- void analytic_delta_level_mappings (const RealVector &level_maps_ref, RealVector &level_maps_new)

  update analytic level mappings; this uses a lightweight approach for incremental statistics (no derivatives, no final-Statistics update)
- void config_integration (unsigned short quad_order, unsigned short ssg_level, const RealVector &dim_pref, short u_space_type, Iterator &u_space_sampler, Model &g_u_model)

  configure u_space_sampler based on numerical integration specification
- void config_integration (short exp_coeffs_approach, unsigned short num_int, const RealVector &dim_pref, Iterator &u_space_sampler, Model &g_u_model)

  configure u_space_sampler based on expansion coefficients approach
- void config_approximation_type (String &approx_type)

  define approx_type based on expansion settings

Private Attributes

- RealVector deltaRespMean

  change in response means induced by a refinement candidate
- RealVector deltaRespVariance

  change in (DIAGONAL) response variance induced by a refinement candidate
- RealSymMatrix deltaRespCovariance

  change in (FULL) response covariance induced by a refinement candidate
- RealVector deltaLevelMaps

  change in response means induced by a refinement candidate

Additional Inherited Members

14.176.1 Detailed Description

Nonintrusive stochastic collocation approaches to uncertainty quantification.

The NonDStochCollocation class uses a stochastic collocation (SC) approach to approximate the effect of parameter uncertainties on response functions of interest. It utilizes the InterpPolyApproximation class to manage multidimensional Lagrange polynomial interpolants.

14.176.2 Constructor & Destructor Documentation

14.176.2.1 NonDStochCollocation (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation using the ProblemDescDB.

References Response::active_set(), Model::assign_rep(), ParallelLibrary::command_line_check(), NonDStochCollocation::config_approximation_type(), NonDStochCollocation::config_integration(), NonDExpansion::construct_expansion_sampler(), Model::current_response(), ActiveSet::derivative_vector(), ProblemDescDB::get_bool(), ProblemDescDB::get_iv(), ProblemDescDB::get_rv(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), ProblemDescDB::get_ushort(), NonDStochCollocation::initialize_u_space_model(), Iterator::iteratedModel, NonDExpansion::numSamplesOnModel, Iterator::outputLevel, Iterator::parallelLib, Iterator::probDescDB, Model::qoi(), NonDStochCollocation::resolve_inputs(), and NonDExpansion::uSpaceModel.

14.176.2.2 NonDStochCollocation (Model & *model,* short *exp_coeffs_approach,* unsigned short *num_int,* const RealVector & *dim_pref,* short *u_space_type,* short *refine_type,* short *refine_control,* short *covar_control,* short *rule_nest,* short *rule_growth,* bool *piecewise_basis,* bool *use_derivs*)

alternate constructor

This constructor is used for helper iterator instantiation on the fly.

References Response::active_set(), Model::assign_rep(), NonDStochCollocation::config_approximation_type(), NonDStochCollocation::config_integration(), Model::current_response(), ActiveSet::derivative_vector(), NonDStochCollocation::initialize_u_space_model(), Iterator::iteratedModel, Iterator::outputLevel, Model::qoi(), NonDStochCollocation::resolve_inputs(), and NonDExpansion::uSpaceModel.

14.176.2.3 NonDStochCollocation (unsigned short *method_name,* ProblemDescDB & *problem_db,* Model & *model*) [protected]

short-cut ctor allowing derived class to replace logic in base class ctor (method_name is not necessary, rather it is just a convenient overload allowing the derived ML SC class to bypass the standard SC ctor)

This constructor is called from derived class constructors that customize the object construction.

14.176.2.4 NonDStochCollocation (unsigned short *method_name,* Model & *model,* short *exp_coeffs_approach,* const RealVector & *dim_pref,* short *refine_type,* short *refine_control,* short *covar_control,* short *ml_alloc_control,* short *ml_discrep,* short *rule_nest,* short *rule_growth,* bool *piecewise_basis,* bool *use_derivs*) [protected]

short-cut ctor allowing derived class to replace logic in base class ctor

This constructor is called from derived class constructors that customize the object construction.

References NonDExpansion::multilevAllocControl, and NonDExpansion::multilevDiscrepEmulation.

14.176.3 Member Function Documentation

14.176.3.1 Real compute_covariance_metric (bool *revert,* bool *print_metric*) [protected], [virtual]

compute 2-norm of change in response covariance

computes the default refinement metric based on change in respCovariance

Reimplemented from NonDExpansion.

References NonDExpansion::compute_covariance_metric(), NonDStochCollocation::compute_delta_covariance(), NonDStochCollocation::compute_delta_mean(), NonDStochCollocation::compute_delta_variance(), NonDExpansion::covarianceControl, NonDStochCollocation::deltaRespCovariance, NonDStochCollocation::delta-

RespVariance, NonDExpansion::expansionBasisType, NonDExpansion::relativeMetric, NonDExpansion::resp-Covariance, and NonDExpansion::respVariance.

14.176.3.2 Real compute_level_mappings_metric (bool *revert,* bool *print_metric*) [protected], [virtual]

compute 2-norm of change in final statistics

computes a "goal-oriented" refinement metric employing computed∗Levels

Reimplemented from NonDExpansion.

References NonDExpansion::allVars, NonDStochCollocation::analytic_delta_level_mappings(), Model::approximations(), NonD::cdfFlag, NonDStochCollocation::compute_delta_covariance(), NonDStochCollocation::compute_delta_-mean(), NonDStochCollocation::compute_delta_variance(), NonDExpansion::compute_level_mappings_metric(), NonDExpansion::compute_numerical_level_mappings(), NonDExpansion::covarianceControl, NonDStoch-Collocation::deltaLevelMaps, NonDExpansion::expansionBasisType, NonDExpansion::initialPtU, Analyzer::num-Functions, NonD::print_level_mappings(), NonD::pull_level_mappings(), NonD::push_level_mappings(), NonD-Expansion::refineMetric, NonDExpansion::relativeMetric, NonD::requestedGenRelLevels, NonD::requestedProb-Levels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, NonDExpansion::stats-MetricMode, NonD::totalLevelRequests, and NonDExpansion::uSpaceModel.

14.176.3.3 void analytic_delta_level_mappings (const RealVector & *level_maps_ref,* RealVector & *level_maps_new*) [protected]

update analytic level mappings; this uses a lightweight approach for incremental statistics (no derivatives, no final-Statistics update)

In this function, we leave numerical stats alone, updating analytic level stats either using ref+delta or, if ref is invalid, though recomputation.

References NonDExpansion::allVars, Model::approximations(), NonD::cdfFlag, NonDStochCollocation::deltaLevel-Maps, NonDExpansion::initialPtU, Analyzer::numFunctions, NonD::requestedGenRelLevels, NonD::requestedProb-Levels, NonD::requestedRelLevels, NonD::requestedRespLevels, NonD::respLevelTarget, NonDExpansion::stats-MetricMode, NonD::totalLevelRequests, and NonDExpansion::uSpaceModel.

Referenced by NonDStochCollocation::compute_level_mappings_metric().

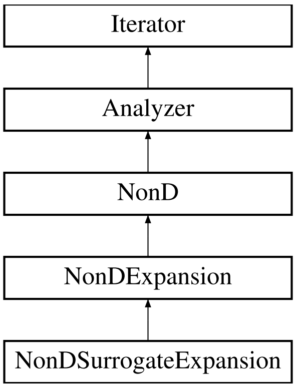
The documentation for this class was generated from the following files:

- NonDStochCollocation.hpp
- NonDStochCollocation.cpp

14.177 NonDSurrogateExpansion Class Reference

Generic uncertainty quantification with Model-based stochastic expansions.

Inheritance diagram for NonDSurrogateExpansion:



Public Member Functions

- NonDSurrogateExpansion (ProblemDescDB &problem_db, Model &model)
    standard constructor
- ∼NonDSurrogateExpansion ()
    destructor

Protected Member Functions

- void **print_results** (std::ostream &)

Additional Inherited Members

14.177.1 Detailed Description

Generic uncertainty quantification with Model-based stochastic expansions.

The NonDSurrogateExpansion class leverages a Model specification for stochastic expansions (PCE, SC, FT) to build a stochastic emulator and then queries the emulator to generate the set of requested statistics.

14.177.2 Constructor & Destructor Documentation

14.177.2.1 NonDSurrogateExpansion (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation using the ProblemDescDB.

References Dakota::abort_handler(), NonDExpansion::construct_expansion_sampler(), ProblemDescDB::get_bool(), ProblemDescDB::get_iv(), ProblemDescDB::get_string(), ProblemDescDB::get_ushort(), Iterator::iteratedModel, Model::model_type(), Iterator::probDescDB, Model::surrogate_type(), and NonDExpansion::uSpaceModel.

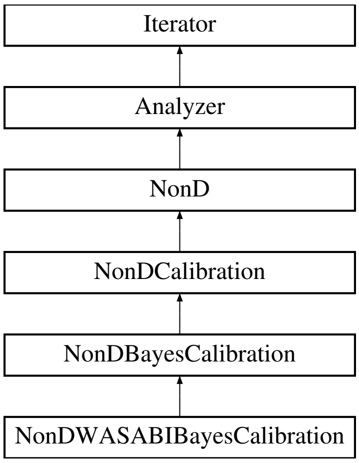
The documentation for this class was generated from the following files:

- NonDSurrogateExpansion.hpp
- NonDSurrogateExpansion.cpp

14.178 NonDWASABIBayesCalibration Class Reference

WASABI - Weighted Adaptive Surrogate Approximations for Bayesian Inference.

Inheritance diagram for NonDWASABIBayesCalibration:



Public Member Functions

- NonDWASABIBayesCalibration (ProblemDescDB &problem_db, Model &model)

    standard constructor
- ∼NonDWASABIBayesCalibration ()

    destructor
- void **compute_responses** (RealMatrix &samples, RealMatrix &responses)

Static Public Member Functions

- static void problem_size (int &chain_num, int &cr_num, int &gen_num, int &pair_num, int &par_num)

    initializer for problem size characteristics in WASABI
- static void problem_value (std::string ∗chain_filename, std::string ∗gr_filename, double &gr_threshold, int &jumpstep, double limits[ ], int par_num, int &printstep, std::string ∗restart_read_filename, std::string ∗restart-_write_filename)

    Filename and data initializer for WASABI.

Protected Member Functions

- void calibrate () override
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS) override

    print the final iterator results
- void compute_statistics () override

    Compute final stats for MCMC chains.
- void extract_selected_posterior_samples (const std::vector< int > &points_to_keep, const RealMatrix &samples_for_posterior_eval, const RealVector &posterior_density, RealMatrix &posterior_data) const

    Extract a subset of samples for posterior eval according to the indices in points_to_keep.
- void export_posterior_samples_to_file (const std::string filename, const RealMatrix &posterior_data) const

    Export posterior_data to file.

Protected Attributes

- int numPushforwardSamples

    number of samples from the prior that is pushed forward through the model

- RealVector dataDistMeans

  The mean of the multivariate Gaussian distribution of the obs. data.
- RealVector dataDistCovariance

  The covariance of the multivariate Gaussian distribution of the obs. data.
- std::string dataDistFilename

  The filename of the file containing the data that with density estimator defines the distribution of the obs. data.
- std::string dataDistCovType

  The type of covariance data provided ("diagonal","matrix")
- std::string posteriorSamplesImportFile

  The filename of the import file containing samples at which the posterior will be evaluated.
- unsigned short posteriorSamplesImportFormat

  Format of imported posterior samples file.
- std::string exportPosteriorDensityFile

  The filename of the export file containing an arbitrary set of samples and their corresponding density values.
- std::string exportPosteriorSamplesFile

  The filename of the export file containing samples from the posterior and their corresponding density values.
- unsigned short exportFileFormat

  Format of imported posterior samples and values file.
- bool generateRandomPosteriorSamples

  Flag specifying whether to generate random samples from the posterior.
- bool evaluatePosteriorDensity

  Flag specifying whether to evaluate the posterior density at a set of samples.
- RealVector paramMins

  lower bounds on calibrated parameters
- RealVector paramMaxs

  upper bounds on calibrated parameters
- boost::mt19937 rnumGenerator

  random number engine for sampling the prior
- RealMatrix momentStatistics

  Matrix for moment statistics. Note that posterior values have density associated with them so we can't use the compute_moments in NonDSampling.

Additional Inherited Members

14.178.1 Detailed Description

WASABI - Weighted Adaptive Surrogate Approximations for Bayesian Inference.

This class performs Bayesian calibration using the WASABI approach

14.178.2 Constructor & Destructor Documentation

14.178.2.1 NonDWASABIBayesCalibration (ProblemDescDB & *problem_db*, Model & *model*)

standard constructor

This constructor is called for a standard letter-envelope iterator instantiation. In this case, set_db_list_nodes has been called and probDescDB can be queried for settings from the method specification.

14.178.3 Member Function Documentation

14.178.3.1 void calibrate ( ) [override], [protected], [virtual]

Perform the uncertainty quantification

Implements NonDBayesCalibration.

References Dakota::abort_handler(), Dakota::copy_data(), NonDWASABIBayesCalibration::dataDistCovariance, NonDWASABIBayesCalibration::dataDistFilename, NonDWASABIBayesCalibration::dataDistMeans, NonDBayesCalibration::emulatorType, NonDWASABIBayesCalibration::evaluatePosteriorDensity, NonDWASABIBayesCalibration::export_posterior_samples_to_file(), NonDWASABIBayesCalibration::exportPosteriorDensityFile, NonDWASABIBayesCalibration::exportPosteriorSamplesFile, NonDWASABIBayesCalibration::extract_selected_posterior_samples(), Dakota::generate_system_seed(), NonDWASABIBayesCalibration::generateRandomPosteriorSamples, NonDBayesCalibration::mcmcModel, NonDWASABIBayesCalibration::momentStatistics, Model::multivariate_distribution(), Analyzer::numContinuousVars, Analyzer::numFunctions, NonDWASABIBayesCalibration::numPushforwardSamples, Iterator::outputLevel, NonDWASABIBayesCalibration::paramMaxs, NonDWASABIBayesCalibration::paramMins, NonDWASABIBayesCalibration::posteriorSamplesImportFile, NonDBayesCalibration::prior_density(), NonDBayesCalibration::prior_sample(), NonDBayesCalibration::randomSeed, Dakota::read_unsized_data(), and NonDWASABIBayesCalibration::rnumGenerator.

14.178.3.2 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [override], [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from NonDBayesCalibration.

References Model::current_response(), Response::function_labels(), NonDBayesCalibration::mcmcModel, NonDWASABIBayesCalibration::momentStatistics, and NonDSampling::print_moments().

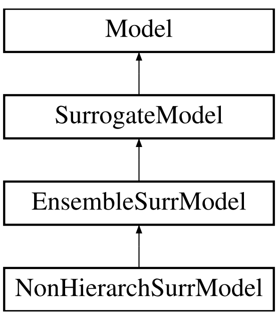
The documentation for this class was generated from the following files:

- NonDWASABIBayesCalibration.hpp
- NonDWASABIBayesCalibration.cpp

14.179 NonHierarchSurrModel Class Reference

Derived model class within the surrogate model branch for managing unordered surrogate models of varying fidelity.

Inheritance diagram for NonHierarchSurrModel:



Public Member Functions

- NonHierarchSurrModel (ProblemDescDB &problem_db)

constructor
- ∼NonHierarchSurrModel ()

  destructor

Protected Member Functions

- bool initialize_mapping (ParLevLIter pl_iter)
- bool finalize_mapping ()
- void derived_evaluate (const ActiveSet &set)
- void derived_evaluate_nowait (const ActiveSet &set)
- void **derived_synchronize_sequential** (IntResponseMapArray &model_resp_maps_rekey, bool block)
- void **derived_synchronize_combine** (IntResponseMapArray &model_resp_maps, IntResponseMap &combined_resp_map)
- void **derived_synchronize_combine_nowait** (IntResponseMapArray &model_resp_maps, IntResponseMap &combined_resp_map)
- void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

  set primaryA{C,DI,DS,DR}VarMapIndices, secondaryA{C,DI,DS,DR}VarMapTargets (coming from a higher-level NestedModel context to inform derivative est.)
- void create_tabular_datastream ()

  create a tabular output stream for automatic logging of vars/response data
- void derived_auto_graphics (const Variables &vars, const Response &resp)

  Update tabular/graphics data with latest variables/response data.
- size_t num_approximation_models () const

  return the number of models that approximate the truth model
- void assign_default_keys ()

  initialize truth and surrogate model keys to default values
- void resize_maps ()

  size id_maps and cached_resp_maps arrays according to responseMode
- void resize_response (bool use_virtual_counts=true)

  resize currentResponse based on responseMode
- size_t insert_response_start (size_t position)

  compute start index for inserting response data into aggregated response
- void insert_metadata (const RealArray &md, size_t position, Response &agg_response)

  insert a single response into an aggregated response in the specified position
- Model & surrogate_model (size_t i=_NPOS)

  return the indexed approximate model from unorderedModels
- const Model & surrogate_model (size_t i=_NPOS) const

  return the indexed approximate model from unorderedModels
- Model & truth_model ()

  return the high fidelity model
- const Model & truth_model () const

  return the high fidelity model
- void active_model_key (const Pecos::ActiveKey &key)

  define the active model key
- void clear_model_keys ()

  remove keys for any approximations underlying {truth,unordered}Models
- void derived_subordinate_models (ModelList &ml, bool recurse_flag)

  return orderedModels and, optionally, their sub-model recursions
- void resize_from_subordinate_model (size_t depth=SZ_MAX)

  resize currentResponse if needed when one of the subordinate models has been resized

- void update_from_subordinate_model (size_t depth=SZ_MAX)

    update currentVariables using non-active data from the passed model (one of the ordered models)
- void primary_response_fn_weights (const RealVector &wts, bool recurse_flag=true)

    set the relative weightings for multiple objective functions or least squares terms and optionally recurses into LF/HF models
- void component_parallel_mode (short mode)

    update component parallel mode for supporting parallelism in the low ad high fidelity models
- IntIntPair estimate_partition_bounds (int max_eval_concurrency)

    estimate the minimum and maximum partition sizes that can be utilized by this Model
- void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

    set up parallel operations for the array of ordered model fidelities
- void derived_init_serial ()

    set up serial operations for the array of ordered model fidelities
- void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

    set active parallel configuration within the current low and high fidelity models identified by {low,high}FidelityKey
- void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

    deallocate communicator partitions for the NonHierarchSurrModel (request forwarded to the the array of ordered model fidelities)
- void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)

    Service the low and high fidelity model job requests received from the master; completes when termination message received from stop_servers().
- void inactive_view (short view, bool recurse_flag=true)

    update the Model's inactive view based on higher level (nested) context and optionally recurse into
- bool evaluation_cache (bool recurse_flag=true) const

    if recurse_flag, return true if orderedModels evaluation cache usage
- bool restart_file (bool recurse_flag=true) const

    if recurse_flag, return true if orderedModels restart file usage
- void fine_grained_evaluation_counters ()

    request fine-grained evaluation reporting within the low and high fidelity models
- void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const

    print the evaluation summary for the NonHierarchSurrModel (request forwarded to the low and high fidelity models)
- void warm_start_flag (const bool flag)

    set the warm start flag, including the orderedModels

Private Member Functions

- void assign_key (const Pecos::ActiveKey &key)

    assign the resolution level for the model form indicated by the key
- void assign_key (size_t i)

    assign the resolution level for the i-th model key
- bool matching_truth_surrogate_interface_ids ()

    check for matching interface ids among active truth/surrogate models (varies based on active keys)
- bool matching_all_interface_ids ()

    check for matching interface ids across full set of models (invariant)
- void check_model_interface_instance ()

    update sameInterfaceInstance based on interface ids for models identified by current {low,high}FidelityKey
- void stop_model (short model_id)

    stop the servers for the model instance identified by the passed id
- bool test_asv (const ShortArray &asv)

    check whether incoming ASV has any active content

Private Attributes

- Model truthModel

  the single truth reference model
- ModelArray unorderedModels

  unordered set of model approximations
- std::vector< Pecos::ActiveKey > surrModelKeys

  keys defining model forms / resolution levels for the active set of approximations

Additional Inherited Members

14.179.1 Detailed Description

Derived model class within the surrogate model branch for managing unordered surrogate models of varying fidelity.

The NonHierarchSurrModel class manages a set of models of varying fidelity. The class contains an unordered array of approximation models, where each model form may also contain a set of solution levels (space/time discretization, convergence tolerances, etc.).

14.179.2 Member Function Documentation

14.179.2.1 bool initialize_mapping (ParLevLIter *pl_iter*) [protected], [virtual]

Inactive variables must be propagated when a NonHierarchSurrModel is employed by a sub-iterator (e.g., OUU with MLMC or MLPCE). In current use cases, this can occur once per sub-iterator execution within Model::initialize_-mapping().

Reimplemented from Model.

References EnsembleSurrModel::init_model(), Model::initialize_mapping(), NonHierarchSurrModel::truthModel, and NonHierarchSurrModel::unorderedModels.

14.179.2.2 bool finalize_mapping ( ) [protected], [virtual]

Inactive variables must be propagated when a NonHierarchSurrModel is employed by a sub-iterator (e.g., OUU with MLMC or MLPCE). In current use cases, this can occur once per sub-iterator execution within Model::initialize_-mapping().

Reimplemented from Model.

References Model::finalize_mapping(), NonHierarchSurrModel::truthModel, and NonHierarchSurrModel-::unorderedModels.

14.179.2.3 void derived_evaluate (const ActiveSet & *set*) [protected], [virtual]

Compute the response synchronously using LF model, HF model, or both (mixed case). For the LF model portion, compute the high fidelity response if needed with build_approximation(), and, if correction is active, correct the low fidelity results.

Reimplemented from Model.

References Dakota::abort_handler(), Response::active_set(), NonHierarchSurrModel::assign_key(), Surrogate-Model::asv_split(), NonHierarchSurrModel::component_parallel_mode(), Model::current_response(), Model-::currentResponse, Model::evaluate(), SurrogateModel::insert_response(), EnsembleSurrModel::qoi(), ActiveSet-::request_vector(), SurrogateModel::responseMode, EnsembleSurrModel::sameModelInstance, SurrogateModel-::surrModelEvalCntr, NonHierarchSurrModel::test_asv(), NonHierarchSurrModel::truthModel, EnsembleSurrModel-::truthModelKey, NonHierarchSurrModel::unorderedModels, Response::update(), and SurrogateModel::update_-model().

14.179.2.4 void derived_evaluate_nowait (const ActiveSet & *set*) [protected], [virtual]

Compute the response asynchronously using LF model, HF model, or both (mixed case). For the LF model portion, compute the high fidelity response with build_approximation() (for correcting the low fidelity results in derived_-synchronize() and derived_synchronize_nowait()) if not performed previously.

Reimplemented from Model.

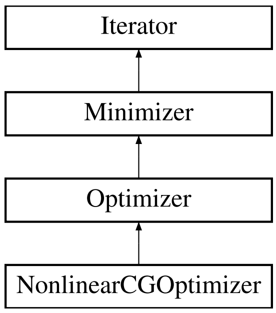
References Dakota::abort_handler(), NonHierarchSurrModel::assign_key(), SurrogateModel::asv_split(), Model-::asynch_flag(), EnsembleSurrModel::cachedRespMaps, NonHierarchSurrModel::component_parallel_mode(), Response::copy(), Model::current_response(), Model::evaluate(), Model::evaluate_nowait(), Model::evaluation_id(), EnsembleSurrModel::modelIdMaps, EnsembleSurrModel::qoi(), ActiveSet::request_vector(), SurrogateModel-::responseMode, EnsembleSurrModel::sameModelInstance, SurrogateModel::surrModelEvalCntr, NonHierarch-SurrModel::test_asv(), NonHierarchSurrModel::truthModel, EnsembleSurrModel::truthModelKey, NonHierarchSurr-Model::unorderedModels, and SurrogateModel::update_model().

The documentation for this class was generated from the following files:

- NonHierarchSurrModel.hpp
- NonHierarchSurrModel.cpp

14.180 NonlinearCGOptimizer Class Reference

Inheritance diagram for NonlinearCGOptimizer:



Public Member Functions

- NonlinearCGOptimizer (ProblemDescDB &problem_db, Model &model)

  standard constructor
- ∼NonlinearCGOptimizer ()

  destructor
- Real linesearch_eval (const Real &trial_step, short req_val=1)

  evaluate the objective function given a particular step size (public for use in boost_ls_eval functor; could use friend)

Protected Member Functions

- void core_run ()

  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Private Member Functions

- void parse_options ()

  constructor helper function to parse misc_options from ProblemDescDB

- void compute_direction ()

  compute next direction via choice of method
- bool compute_step ()

  compute step: fixed, simple decrease, sufficient decrease
- void bracket_min (Real &xa, Real &xb, Real &xc, Real &fa, Real &fb, Real &fc)

  bracket the 1-D minimum in the linesearch
- Real brent_minimize (Real a, Real b, Real tol)

  Perform 1-D minimization for the stepLength using Brent's method.

Private Attributes

- Real initialStep

  initial step length
- Real linesearchTolerance

  approximate accuracy of absissca in LS
- unsigned linesearchType

  type of line search (if any)
- unsigned maxLinesearchIters

  maximum evaluations in line search
- Real relFunctionTol

  stopping criterion for rel change in fn
- Real relGradientTol

  stopping criterion for rel reduction in g
- bool resetStep

  whether to reset step with each linesearch
- unsigned restartIter

  iter at which to reset to steepest descent
- unsigned updateType

  type of CG direction update
- unsigned iterCurr

  current iteration number
- RealVector designVars

  current decision variables in the major iteration
- RealVector trialVars

  decision variables in the linesearch
- Real functionCurr

  current function value
- Real functionPrev

  previous function value
- RealVector gradCurr

  current gradient
- RealVector gradPrev

  previous gradient
- RealVector gradDiff

  temporary for gradient difference (gradCurr - gradPrev)
- RealVector searchDirection

  current aggregate search direction
- Real stepLength

  current step length parameter alpha
- Real gradDotGrad_init

initial gradient norm squared

- Real gradDotGrad_curr

  gradCurr dot gradCurr

- Real gradDotGrad_prev

  gradPrev dot gradPrev

Additional Inherited Members

14.180.1 Detailed Description

Experimental implementation of nonlinear CG optimization

14.180.2 Member Function Documentation

14.180.2.1 void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Iterator::activeSet, Iterator::bestResponseArray, Iterator::bestVariablesArray, NonlinearCGOptimizer::compute_direction(), NonlinearCGOptimizer::compute_step(), Model::continuous_variables(), Iterator::convergenceTol, Dakota::copy_data(), Model::current_response(), NonlinearCGOptimizer::designVars, Model::evaluate(), Response::function_gradient_copy(), Response::function_gradient_view(), Response::function_values(), NonlinearCGOptimizer::functionCurr, NonlinearCGOptimizer::functionPrev, NonlinearCGOptimizer::gradCurr, NonlinearCGOptimizer::gradDotGrad_curr, NonlinearCGOptimizer::gradDotGrad_init, NonlinearCGOptimizer::gradDotGrad_prev, NonlinearCGOptimizer::gradPrev, Iterator::iteratedModel, NonlinearCGOptimizer::iterCurr, NonlinearCGOptimizer::linesearchType, Optimizer::localObjectiveRecast, Iterator::maxIterations, Minimizer::numContinuousVars, Iterator::outputLevel, NonlinearCGOptimizer::relFunctionTol, NonlinearCGOptimizer::relGradientTol, ActiveSet::request_values(), NonlinearCGOptimizer::searchDirection, NonlinearCGOptimizer::stepLength, and NonlinearCGOptimizer::trialVars.

14.180.2.2 Real brent_minimize (Real *a*, Real *b*, Real *tol*) [private]

Perform 1-D minimization for the stepLength using Brent's method.

Perform 1-D minimization for the stepLength using Brent's method. This is a C translation of fmin.f from Netlib.

References NonlinearCGOptimizer::linesearch_eval(), NonlinearCGOptimizer::maxLinesearchIters, and Iterator::outputLevel.

Referenced by NonlinearCGOptimizer::compute_step().

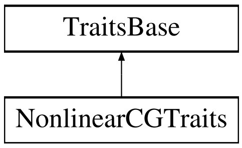
The documentation for this class was generated from the following files:

- NonlinearCGOptimizer.hpp
- NonlinearCGOptimizer.cpp

14.181 NonlinearCGTraits Class Reference

A version of TraitsBase specialized for NonlinearCG optimizers.

Inheritance diagram for NonlinearCGTraits:



Public Member Functions

- NonlinearCGTraits ()

  default constructor
- virtual ~NonlinearCGTraits ()

  destructor
- virtual bool is_derived ()

  A temporary query used in the refactor.
- bool supports_continuous_variables ()

  Return the flag indicating whether method supports continuous variables.

14.181.1 Detailed Description

A version of TraitsBase specialized for NonlinearCG optimizers.

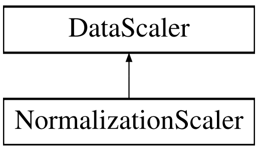
The documentation for this class was generated from the following file:

- NonlinearCGOptimizer.hpp

14.182 NormalizationScaler Class Reference

Normalizes the data using max and min feature values.

Inheritance diagram for NormalizationScaler:



Public Member Functions

- NormalizationScaler (const MatrixXd &features, bool mean_normalization, double norm_factor=1.0)

  Main constructor for NormalizationScaler.

Additional Inherited Members

14.182.1 Detailed Description

Normalizes the data using max and min feature values.

if (mean_normalization): scaler_offsets = mean else: scaler_offsets = min

scale_factors = (max - min)/norm_factor

Setting mean_normalization = false scales each feature to [0,1]

14.182.2 Constructor & Destructor Documentation

14.182.2.1 NormalizationScaler (const MatrixXd & *features*, bool *mean_normalization*, double *norm_factor* = `1.0`)

Main constructor for NormalizationScaler.

Parameters

`in`	*features*	Unscaled data matrix - (num_samples by num_features)
`in`	*mean_-normalization*	Flag for whether to use mean or min value as the offset
`in`	*norm_factor*	Optional scaling factor applied to each feature Has a default value of 1.0

References DataScaler::hasScaling, DataScaler::scaledSample, DataScaler::scalerFeaturesOffsets, and DataScaler::scalerFeaturesScaleFactors.

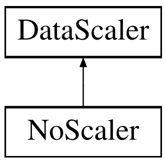
The documentation for this class was generated from the following files:

- UtilDataScaler.hpp
- UtilDataScaler.cpp

14.183 NoScaler Class Reference

Leaves the data unscaled.

Inheritance diagram for NoScaler:



Public Member Functions

- NoScaler (const MatrixXd &features)

  Main constructor for NoScaler.

Additional Inherited Members

14.183.1 Detailed Description

Leaves the data unscaled.

This DataScaler has fixed coefficients that amount to an identity operation. It is useful when the data has already been scaled or scaling is desired.

scaler_offsets = 0.0

scale_factors = 1.0

14.183.2 Constructor & Destructor Documentation

14.183.2.1 NoScaler (const MatrixXd & *features*)

Main constructor for NoScaler.

Parameters

in	*features*	Unscaled data matrix - (num_samples by num_features)

References DataScaler::hasScaling, DataScaler::scaledSample, DataScaler::scalerFeaturesOffsets, and DataScaler::scalerFeaturesScaleFactors.

The documentation for this class was generated from the following files:

- UtilDataScaler.hpp
- UtilDataScaler.cpp

14.184 NOWPACBlackBoxEvaluator Class Reference

Derived class for plugging Dakota evaluations into NOWPAC solver.

Inherits BlackBoxBaseClass.

Public Member Functions

- NOWPACBlackBoxEvaluator (Model &model)

  constructor
- void **evaluate** (std::vector< double > const &x, std::vector< double > &vals, void ∗param)
- void **evaluate** (std::vector< double > const &x, std::vector< double > &vals, std::vector< double > &noise, void ∗param)
- double **evaluate_samples** (std::vector< double > const &samples, const unsigned int index, std::vector< double >const &x)
- void **allocate_constraints** ()
- int **num_ineq_constraints** () const
- const SizetList & **nonlinear_inequality_mapping_indices** () const
- const RealList & **nonlinear_inequality_mapping_multipliers** () const
- const RealList & **nonlinear_inequality_mapping_offsets** () const
- void set_unscaled_bounds (const RealVector &l_bnds, const RealVector &u_bnds)

  set {lower,upper}Bounds
- void scale (const RealVector &unscaled_x, RealArray &scaled_x) const

  perform scaling from [lower,upper] to [0,1]
- void unscale (const RealArray &scaled_x, RealVector &unscaled_x) const

  invert scaling to return from [0,1] to [lower,upper]

Private Attributes

- Model iteratedModel

  cache a local copy of the Model
- RealVector lowerBounds

  cache the active continuous lower bounds for scaling to [0,1]
- RealVector upperBounds

  cache the active continuous upper bounds for scaling to [0,1]
- int numNowpacIneqConstr

  aggregate unsupported constraint types as nonlinear inequalities
- SizetList nonlinIneqConMappingIndices

  a list of indices for referencing the DAKOTA nonlinear inequality constraints used in computing the corresponding NOWPAC constraints.
- RealList nonlinIneqConMappingMultipliers

a list of multipliers for mapping the DAKOTA nonlinear inequality constraints to the corresponding NOWPAC constraints.
- RealList nonlinIneqConMappingOffsets

  a list of offsets for mapping the DAKOTA nonlinear inequality constraints to the corresponding NOWPAC constraints.
- SizetList linIneqConMappingIndices

  a list of indices for referencing the DAKOTA linear inequality constraints used in computing the corresponding NOWPAC constraints.
- RealList linIneqConMappingMultipliers

  a list of multipliers for mapping the DAKOTA linear inequality constraints to the corresponding NOWPAC constraints.
- RealList linIneqConMappingOffsets

  a list of offsets for mapping the DAKOTA linear inequality constraints to the corresponding NOWPAC constraints.

14.184.1 Detailed Description

Derived class for plugging Dakota evaluations into NOWPAC solver.

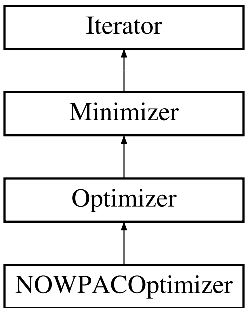
The documentation for this class was generated from the following files:

- NOWPACOptimizer.hpp
- NOWPACOptimizer.cpp

14.185 NOWPACOptimizer Class Reference

Wrapper class for the (S)NOWPAC optimization algorithms from Florian Augustin (MIT)

Inheritance diagram for NOWPACOptimizer:



Public Member Functions

- NOWPACOptimizer (ProblemDescDB &problem_db, Model &model)

  standard constructor
- NOWPACOptimizer (Model &model)

  alternate constructor
- ∼NOWPACOptimizer ()

  destructor
- void core_run ()

  core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Private Member Functions

- void initialize_options ()

  Shared constructor code.

Private Attributes

- NOWPAC **nowpacSolver**
- NOWPACBlackBoxEvaluator **nowpacEvaluator**

Additional Inherited Members

14.185.1 Detailed Description

Wrapper class for the (S)NOWPAC optimization algorithms from Florian Augustin (MIT)

14.185.2 Member Function Documentation

14.185.2.1 void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Iterator::bestResponseArray, Iterator::bestVariablesArray, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variables(), Iterator::iteratedModel, Optimizer::localObjectiveRecast, Minimizer::numContinuousVars, Minimizer::numFunctions, Minimizer::numUserPrimaryFns, Iterator::outputLevel, Model::primary_response_fn_sense(), NOWPACBlackBoxEvaluator::scale(), NOWPACBlackBoxEvaluator::set_unscaled_bounds(), and NOWPACBlackBoxEvaluator::unscale().

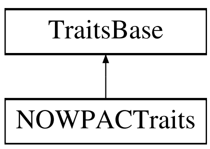
The documentation for this class was generated from the following files:

- NOWPACOptimizer.hpp
- NOWPACOptimizer.cpp

14.186 NOWPACTraits Class Reference

A version of TraitsBase specialized for NOWPAC optimizers.

Inheritance diagram for NOWPACTraits:



Public Member Functions

- NOWPACTraits ()

    default constructor
- virtual ∼NOWPACTraits ()

    destructor
- virtual bool is_derived ()

    A temporary query used in the refactor.
- bool supports_continuous_variables ()

    Return the flag indicating whether method supports continuous variables.

- bool supports_linear_inequality ()

  Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_inequality ()

  Return the flag indicating whether method supports nonlinear inequalities.
- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()

  Return the format used for nonlinear inequality constraints.

14.186.1 Detailed Description

A version of TraitsBase specialized for NOWPAC optimizers.

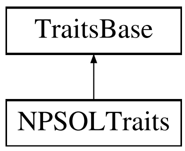
The documentation for this class was generated from the following file:

- NOWPACOptimizer.hpp

14.187 NPSOLTraits Class Reference

Wrapper class for the NPSOL optimization library.

Inheritance diagram for NPSOLTraits:



Public Member Functions

- NPSOLTraits ()

  default constructor
- virtual ∼NPSOLTraits ()

  destructor
- virtual bool is_derived ()

  A temporary query used in the refactor.
- bool supports_continuous_variables ()

  Return the flag indicating whether method supports continuous variables.
- bool supports_linear_equality ()

  Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()

  Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()

  Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

  Return the flag indicating whether method supports nonlinear inequalities.
- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()

  Return the format used for nonlinear inequality constraints.

14.187.1 Detailed Description

Wrapper class for the NPSOL optimization library.

The NPSOLOptimizer class provides a wrapper for NPSOL, a Fortran 77 sequential quadratic programming library from Stanford University marketed by Stanford Business Associates. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any attribute used within static member functions must be either local to that function or accessed through a static pointer.

The user input mappings are as follows: `max_function_evaluations` is implemented directly in NPSOLOptimizer's evaluator functions since there is no NPSOL parameter equivalent, and `max_iterations`, `convergence_tolerance`, `output` verbosity, `verify_level`, `function_precision`, and `linesearch_tolerance` are mapped into NPSOL's "Major Iteration Limit", "Optimality Tolerance", "Major Print Level" (`verbose`: Major Print Level = 20; `quiet`: Major Print Level = 10), "Verify Level", "Function Precision", and "Linesearch Tolerance" parameters, respectively, using NPSOL's npoptn() subroutine (as wrapped by npoptn2() from the sol_optn_wrapper.f file). Refer to [Gill, P.E., Murray, W., Saunders, M.A., and Wright, M.H., 1986] for information on NPSOL's optional input parameters and the npoptn() subroutine. A version of TraitsBase specialized for NPSOL optimizers

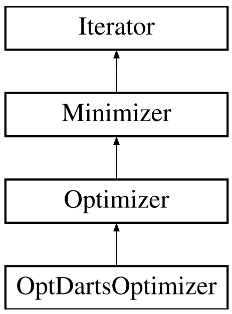
The documentation for this class was generated from the following file:

- NPSOLOptimizer.hpp

14.188 OptDartsOptimizer Class Reference

Wrapper class for OptDarts Optimizer.

Inheritance diagram for OptDartsOptimizer:



Public Member Functions

- OptDartsOptimizer (ProblemDescDB &problem_db, Model &model)

    Constructor.
- OptDartsOptimizer (Model &model)

    alternate constructor for Iterator instantiations by name
- ∼OptDartsOptimizer ()

    Destructor.
- void core_run ()

    Calls the OptDarts algorithm.

Private Member Functions

- void load_parameters (Model &model)

    Convenience function for Parameter loading.

- double opt_darts_f ()

    Function evaluation.
- void opt_darts_execute (size_t num_dim, size_t budget, double ∗xmin, double ∗xmax, double TOL, size_t problem_index, double fw_MC, double fb_MC)

    Run the OPT-DARTS method.
- void opt_darts_initiate (double ∗xmin, double ∗xmax)

    Initialize OPT-DARTS.
- void **opt_darts_reset_convex_hull** ()
- size_t opt_darts_pick_candidate (size_t ifunc)

    Choose the next trial iterate.
- void **retrieve_extended_neighbors** (size_t icandidate)
- void **opt_darts_sample_from_candidate_neighborhood** (size_t icandidate, size_t ifunc)
- void **DIRECT_sample_from_candidate_neighborhood** (size_t icandidate)
- void **opt_darts_add_dart** ()
- void **opt_darts_update_K_h_approximate_Voronoi** (size_t isample)
- void opt_darts_terminate ()

    Release memory and exit cleanly.
- void opt_darts_plot_discs_2d (size_t icandidate)

    Convenience function for plotting iterates.
- void opt_darts_plot_hull_2d (size_t icandidate, size_t ifunc)

    Convenience function for plotting convex hull.
- void **initiate_random_generator** (unsigned long x)
- double **generate_a_random_number** ()
- void **sample_uniformly_from_unit_sphere_surface** (double ∗dart, size_t num_dim)
- bool **trim_line_using_Hyperplane** (size_t num_dim, double ∗st, double ∗end, double ∗qH, double ∗nH)

Private Attributes

- double ∗ **_xmin**
- double ∗ **_xmax**
- double ∗ **_dart**
- double ∗ **_st**
- double ∗ **_end**
- double ∗ **_tmp_point**
- double ∗ **_qH**
- double ∗ **_nH**
- double ∗∗ **_x**
- double ∗∗ **_xc**
- double ∗∗ **_f**
- double ∗∗ **_K**
- double ∗ **_h**
- double ∗ **_r**
- size_t ∗∗ **_neighbors**
- size_t ∗ **_tmp_neighbors**
- size_t ∗ **_ext_neighbors**
- size_t **_num_ext_neighbors**
- bool **_use_opt_darts**
- bool **_estimate_K**
- size_t **_ib**
- size_t **_num_samples**
- size_t **_budget**
- size_t **_num_dim**
- double **_diag**

- size_t **_problem_index**
- double **_fb**
- double **_fw**
- double **_fval**
- size_t **_corner_index**
- size_t **_num_corners**
- size_t * **_corners**
- double **_epsilon**
- double **_fb_MC**
- double **_fw_MC**
- double ** **_xm**
- double ** **_xp**
- double * **_alpha_Deceptive**
- double **Q** [1220]
- int **indx**
- double **cc**
- double **c**
- double **zc**
- double **zx**
- double **zy**
- size_t **qlen**
- bool **use_DIRECT**
- int **numTotalVars**
- int **randomSeed**

Additional Inherited Members

14.188.1 Detailed Description

Wrapper class for OptDarts Optimizer.

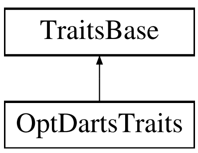
The documentation for this class was generated from the following files:

- OptDartsOptimizer.hpp
- OptDartsOptimizer.cpp

14.189 OptDartsTraits Class Reference

A version of TraitsBase specialized for OptDarts.

Inheritance diagram for OptDartsTraits:



Public Member Functions

- OptDartsTraits ()

    default constructor
- virtual ∼OptDartsTraits ()

    destructor
- virtual bool is_derived ()

    A temporary query used in the refactor.
- bool supports_continuous_variables ()

    Return the flag indicating whether method supports continuous variables.

14.189.1 Detailed Description

A version of TraitsBase specialized for OptDarts.

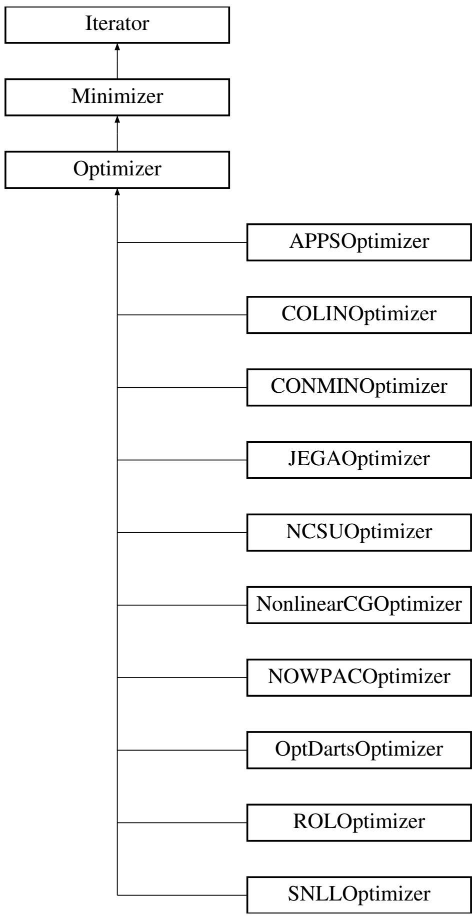
The documentation for this class was generated from the following file:

- OptDartsOptimizer.hpp

14.190 Optimizer Class Reference

Base class for the optimizer branch of the iterator hierarchy.

Inheritance diagram for Optimizer:



Public Member Functions

- void get_common_stopping_criteria (int &max_fn_evals, int &max_iters, double &conv_tol, double &min_var_chg, double &obj_target)
- int **num_nonlin_ineq_constraints_found** () const
- template<typename AdapterT >
  bool get_variable_bounds_from_dakota (typename AdapterT::VecT &lower, typename AdapterT::VecT &upper)
- template<typename VecT >
  void get_responses_from_dakota (const RealVector &dak_fn_vals, VecT &funs, VecT &cEqs, VecT &cIneqs)

Static Public Member Functions

- static void not_available (const std::string &package_name)

  Static helper function: third-party opt packages which are not available.

Protected Member Functions

- Optimizer (std::shared_ptr< TraitsBase > traits)

  default constructor
- Optimizer (ProblemDescDB &problem_db, Model &model, std::shared_ptr< TraitsBase > traits)

  alternate constructor; accepts a model
- Optimizer (unsigned short method_name, Model &model, std::shared_ptr< TraitsBase > traits)

  alternate constructor for "on the fly" instantiations
- Optimizer (unsigned short method_name, size_t num_cv, size_t num_div, size_t num_dsv, size_t num_drv, size_t num_lin_ineq, size_t num_lin_eq, size_t num_nln_ineq, size_t num_nln_eq, std::shared_ptr< TraitsBase > traits)

  alternate constructor for "on the fly" instantiations
- ∼Optimizer ()

  destructor
- void initialize_run ()
- void post_run (std::ostream &s)
- void finalize_run ()

  utility function to perform common operations following post_run(); deallocation and resetting of instance pointers
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)
- void configure_constraint_maps ()
- int **configure_inequality_constraints** (CONSTRAINT_TYPE ctype)
- void **configure_equality_constraints** (CONSTRAINT_TYPE ctype, size_t index_offset)
- template<typename AdapterT >
  void **get_linear_constraints_and_bounds** (typename AdapterT::VecT &lin_ineq_lower_bnds, typename AdapterT::VecT &lin_ineq_upper_bnds, typename AdapterT::VecT &lin_eq_targets, typename AdapterT::MatT &lin_ineq_coeffs, typename AdapterT::MatT &lin_eq_coeffs)

Protected Attributes

- size_t numObjectiveFns

  number of objective functions (iterator view)
- bool localObjectiveRecast

  flag indicating whether local recasting to a single objective is used
- Optimizer ∗ prevOptInstance

  pointer containing previous value of optimizerInstance
- int numNonlinearIneqConstraintsFound

number of nonlinear ineq constraints actually used (based on conditional and bigRealBoundSize

- std::vector< int > constraintMapIndices

  map from Dakota constraint number to APPS constraint number
- std::vector< double > constraintMapMultipliers

  multipliers for constraint transformations
- std::vector< double > constraintMapOffsets

  offsets for constraint transformations

Static Protected Attributes

- static Optimizer * optimizerInstance

  pointer to Optimizer instance used in static member functions

Private Member Functions

- void reduce_model (bool local_nls_recast, bool require_hessians)

  Wrap iteratedModel in a RecastModel that performs (weighted) multi-objective or sum-of-squared residuals transformation.
- void objective_reduction (const Response &full_response, const BoolDeque &sense, const RealVector &full_wts, Response &reduced_response) const

  forward mapping: maps multiple primary response functions to a single weighted objective for single-objective optimizers

Static Private Member Functions

- static void primary_resp_reducer (const Variables &full_vars, const Variables &reduced_vars, const Response &full_response, Response &reduced_response)

  Recast callback to reduce multiple objectives or residuals to a single objective, with gradients and Hessians as needed.

Additional Inherited Members

14.190.1 Detailed Description

Base class for the optimizer branch of the iterator hierarchy.

The Optimizer class provides common data and functionality for DOTOptimizer, CONMINOptimizer, NPSOLOptimizer, SNLLOptimizer, NLPQLPOptimizer, COLINOptimizer, OptDartsOptimizer, NCSUOptimizer, NonlinearCGOptimizer, NomadOptimizer, and JEGAOptimizer.

14.190.2 Member Function Documentation

14.190.2.1 void get_common_stopping_criteria (int & *max_fn_evals,* int & *max_iters,* double & *conv_tol,* double & *min_var_chg,* double & *obj_target*) [inline]

Convenience method for common optimizer stopping criteria vectors

References Iterator::convergenceTol, ProblemDescDB::get_real(), Iterator::maxFunctionEvals, Iterator::maxIterations, and Iterator::probDescDB.

14.190.2.2 bool get_variable_bounds_from_dakota (typename AdapterT::VecT & *lower,* typename AdapterT::VecT & *upper*) [inline]

Method for transferring variable bounds from Dakota data to TPL data

References Minimizer::bigIntBoundSize, Minimizer::bigRealBoundSize, and Iterator::iteratedModel.

14.190.2.3 void get_responses_from_dakota (const RealVector & *dak_fn_vals,* VecT & *funs,* VecT & *cEqs,* VecT & *cIneqs*) [inline]

Method for transferring responses from Dakota data to TPL data

References Optimizer::constraintMapIndices, Optimizer::constraintMapMultipliers, Optimizer::constraintMapOffsets, Dakota::get_responses(), and Iterator::iteratedModel.

Referenced by APPSEvalMgr::recv().

14.190.2.4 void initialize_run ( ) [protected], [virtual]

Implements portions of initialize_run specific to Optimizers. This function should be invoked (or reimplemented) by any derived implementations of initialize_run() (which would otherwise hide it).

Reimplemented from Minimizer.

Reimplemented in SNLLOptimizer, and ROLOptimizer.

References Optimizer::configure_constraint_maps(), Minimizer::initialize_run(), Model::is_null(), Iterator::iteratedModel, Iterator::myModelLayers, Optimizer::optimizerInstance, Optimizer::prevOptInstance, and Model::update_from_subordinate_model().

Referenced by ROLOptimizer::initialize_run(), CONMINOptimizer::initialize_run(), APPSOptimizer::initialize_run(), and SNLLOptimizer::initialize_run().

14.190.2.5 void post_run (std::ostream & *s*) [protected], [virtual]

Implements portions of post_run specific to Optimizers. This function should be invoked (or reimplemented) by any derived implementations of post_run() (which would otherwise hide it).

Reimplemented from Minimizer.

Reimplemented in SNLLOptimizer.

References Dakota::abort_handler(), Iterator::activeSet, Iterator::bestResponseArray, Iterator::bestVariablesArray, Variables::continuous_variables(), Response::function_values_view(), Minimizer::local_recast_retrieve(), Optimizer::localObjectiveRecast, Model::model_rep(), Minimizer::numNonlinearConstraints, Minimizer::numUserPrimaryFns, Minimizer::post_run(), ActiveSet::request_values(), ActiveSet::request_vector(), ScalingModel::resp_scaled2native(), Minimizer::scaleFlag, and Minimizer::scalingModel.

Referenced by COLINOptimizer::post_run(), and SNLLOptimizer::post_run().

14.190.2.6 void finalize_run ( ) [inline], [protected], [virtual]

utility function to perform common operations following post_run(); deallocation and resetting of instance pointers

Optional: perform finalization phases of run sequence, like deallocating memory and resetting instance pointers. Commonly used in sub-iterator executions. This is a virtual function; when re-implementing, a derived class must call its nearest parent's finalize_run(), typically *after* performing its own implementation steps.

Reimplemented from Minimizer.

Reimplemented in SNLLOptimizer.

References Minimizer::finalize_run(), Optimizer::optimizerInstance, and Optimizer::prevOptInstance.

Referenced by SNLLOptimizer::finalize_run().

14.190.2.7 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

Redefines default iterator results printing to include optimization results (objective functions and constraints).

Reimplemented from Iterator.

References Dakota::abort_handler(), Iterator::bestResponseArray, Iterator::bestVariablesArray, Minimizer::calibrationDataFlag, Minimizer::dataTransformModel, Minimizer::expData, Model::interface_id(), Model::model_rep(), ExperimentData::num_config_vars(), Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, Minimizer::numUserPrimaryFns, Minimizer::optimizationFlag, Minimizer::original_model(), Model::primary_response_fn_weights(), Minimizer::print_best_eval_ids(), DataTransformModel::print_best_responses(), Minimizer::print_residuals(), Model::response_size(), Iterator::run_identifier(), and Variables::write().

14.190.2.8 void configure_constraint_maps ( ) [protected]

Implements configuration of constraint maps, etc...

References Dakota::abort_handler(), Minimizer::bigRealBoundSize, Dakota::configure_inequality_constraint_maps(), Optimizer::constraintMapIndices, Optimizer::constraintMapMultipliers, Optimizer::constraintMapOffsets, Iterator::iteratedModel, Optimizer::numNonlinearIneqConstraintsFound, and Iterator::traits().

Referenced by Optimizer::initialize_run().

14.190.2.9 void reduce_model (bool *local_nls_recast*, bool *require_hessians*) [private]

Wrap iteratedModel in a RecastModel that performs (weighted) multi-objective or sum-of-squared residuals transformation.

Reduce model for least-squares or multi-objective transformation. Doesn't map variables, or secondary responses. Maps active set for Gauss-Newton. Maps primary responses to single objective so user vs. iterated matters.

References Iterator::activeSet, Model::assign_rep(), Minimizer::calibrationDataFlag, Model::current_response(), Response::function_gradients(), Iterator::gnewton_set_recast(), Model::hessian_type(), Iterator::iteratedModel, Iterator::myModelLayers, Minimizer::numContinuousVars, Minimizer::numFunctions, Minimizer::numIterPrimaryFns, Minimizer::numNonlinearConstraints, Minimizer::numNonlinearIneqConstraints, Optimizer::numObjectiveFns, Minimizer::numTotalCalibTerms, Minimizer::numUserPrimaryFns, Iterator::outputLevel, Model::primary_fn_type(), Optimizer::primary_resp_reducer(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), ActiveSet::request_vector(), and Response::reshape().

Referenced by Optimizer::Optimizer().

14.190.2.10 void primary_resp_reducer (const Variables & *full_vars*, const Variables & *reduced_vars*, const Response & *full_response*, Response & *reduced_response*) [static], [private]

Recast callback to reduce multiple objectives or residuals to a single objective, with gradients and Hessians as needed.

Objective function map from multiple primary responses (objective or residuals) to a single objective. Currently supports weighted sum; may later want more general transformations, e.g., goal-oriented

References Iterator::iteratedModel, Response::metadata(), SharedResponseData::metadata_labels(), Optimizer::objective_reduction(), Optimizer::optimizerInstance, Iterator::outputLevel, Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), Response::shared_data(), and Model::subordinate_model().

Referenced by Optimizer::reduce_model().

14.190.2.11 void objective_reduction (const Response & *full_response,* const BoolDeque & *sense,* const RealVector & *full_wts,* Response & *reduced_response*) const [private]

forward mapping: maps multiple primary response functions to a single weighted objective for single-objective optimizers

This function is responsible for the mapping of multiple objective functions into a single objective for publishing to single-objective optimizers. Used in DOTOptimizer, NPSOLOptimizer, SNLLOptimizer, and SGOPTApplication on every function evaluation. The simple weighting approach (using primaryRespFnWts) is the only technique supported currently. The weightings are used to scale function values, gradients, and Hessians as needed.

References Response::active_set_request_vector(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian_view(), Response::function_hessians(), Response::function_value(), Response::function_values(), Response::num_functions(), Minimizer::numConstraints, Minimizer::objective(), Minimizer::objective_gradient(), Minimizer::objective_hessian(), Iterator::outputLevel, and Dakota::write_precision.

Referenced by Optimizer::primary_resp_reducer().

The documentation for this class was generated from the following files:

- DakotaOptimizer.hpp
- DakotaOptimizer.cpp

14.191 OutputManager Class Reference

Class to manage redirection of stdout/stderr, keep track of current redir state, and manage rank 0 output. Also manage tabular data output for post-processing with Matlab, Tecplot, etc. and delegate to Graphics for X Windows Graphics.

Public Member Functions

- OutputManager ()

  Default constructor (needed for default environment ctors)
- OutputManager (const ProgramOptions &prog_opts, int dakota_world_rank=0, bool dakota_mpirun_flag=false)

  Standard constructor, taking user-specified program options and optionally taking the rank of this process in Dakota's MPI_Comm.
- ∼OutputManager ()

  Destructor that closes streams and other outputs.
- void close_streams ()

  helper to close streams during destructor or abnormal abort
- Graphics & graphics ()

  retrieve the graphics handler object
- void parse (const ProgramOptions &prog_opts, const ProblemDescDB &problem_db)

  Extract environment options from ProblemDescDB and update from late updates to ProgramOptions.
- void startup_message (const String &start_msg)

  Set the Dakota startup message ("Running on...")
- void push_output_tag (const String &iterator_tag, const ProgramOptions &prog_opts, bool force_cout_redirect, bool force_rst_redirect)

  Update the tag to use on files and rebind any streams as needed.
- String build_output_tag () const

  return the full output tag
- void pop_output_tag ()

  (Potentially) remove an output context and rebind streams
- void output_version (std::ostream &os=Cout) const

Output the current Dakota version.
- void output_startup_message (std::ostream &os=Cout) const

  Output the startup header and time.
- void output_helper (const String &message, std::ostream &os) const

  Output only on Dakota world rank 0 (for version, help, etc.)
- void append_restart (const ParamResponsePair &prp)

  append a parameter/response set to the restart file
- void open_tabular_datastream ()

  open the tabular datastream on iterator leaders
- void create_tabular_header (const Variables &vars, const Response &resp)

  output a complete header to the tabular datastream
- void create_tabular_header (const StringArray &iface_ids)

  initiate the header for the tabular datastream with the leading fields
- void append_tabular_header (const Variables &vars)

  append variables labels to the tabular header
- void append_tabular_header (const Variables &vars, size_t start_index, size_t num_items)

  append a range of variables labels to the tabular header
- void append_tabular_header (const StringArray &labels, bool rtn=false)

  append an array of labels to the tabular header
- void append_tabular_header (const Response &response)

  append response labels to the tabular header
- void add_tabular_data (const Variables &vars, const String &iface, const Response &response)

  adds data to each window in the 2d graphics and adds a row to the tabular data file for the evaluation variables/response
- void add_tabular_data (const Variables &vars)

  adds data to each window in the 2d graphics and adds a row to the tabular data file for the evaluation variables
- void add_tabular_data (const Variables &vars, size_t start_index, size_t num_items)

  adds data to each window in the 2d graphics and adds a row to the tabular data file for a portion of the evaluation variables
- void add_tabular_data (const StringArray &iface_ids)

  adds data to a row of the tabular data file for the interface id
- void add_tabular_data (const Response &response, bool eol=true)

  adds data to each window in the 2d graphics and adds a row to the tabular data file for the response functions
- void add_tabular_data (const Response &response, size_t start_index, size_t num_items)

  adds data to each window in the 2d graphics and adds a row to the tabular data file for a portion of the response functions
- template<class T >
  void add_tabular_scalar (T val)

  augments the data set for a row in the tabular data file
- void add_eol ()

  complete tabular row with EOL
- void close_tabular_datastream ()

  close tabular datastream
- void graphics_counter (int cntr)

  set graphicsCntr equal to cntr
- int graphics_counter () const

  return graphicsCntr
- void tabular_counter_label (const std::string &label)

  set tabularCntrLabel equal to label
- void init_results_db ()

  At runtime, initialize the global ResultsManager, tagging filename with MPI worldRank + 1 if needed.
- void archive_input (const ProgramOptions &prog_opts) const

  Archive the input file to the results database.

Public Attributes

- bool graph2DFlag

  whether user requested 2D graphics plots
- bool tabularDataFlag

  whether user requested tabular data file
- bool resultsOutputFlag

  whether user requested results data output
- String tabularDataFile

  filename for tabulation of graphics data
- String resultsOutputFile

  filename for results data
- unsigned short modelEvalsSelection

  Models selected to store their evaluations.
- unsigned short interfEvalsSelection

  Interfaces selected to store their evaluations.

Private Member Functions

- void initial_redirects (const ProgramOptions &prog_opts)

  Perform initial output/error redirects from user requests.
- void read_write_restart (bool restart_requested, bool read_restart_flag, const String &read_restart_filename, size_t stop_restart_eval, const String &write_restart_filename)

  conditionally import evaluations from restart file, then always create or overwrite restart file

Private Attributes

- int worldRank

  output manager handles rank 0 only output when needed
- bool mpirunFlag

  some output is only for MPI runs
- StringArray fileTags

  set of tags for various input/output files (default none)
- ConsoleRedirector coutRedirector

  set of redirections for Dakota::Cout; stores any tagged filename when there are concurrent Iterators
- ConsoleRedirector cerrRedirector

  set of redirections for Dakota::Cerr; stores any tagged filename when there are concurrent Iterators and error redirection is requested
- std::vector< std::shared_ptr
  < RestartWriter > > restartDestinations

  Stack of active restart destinations; end is the last (active) redirection. All remain open until popped or destroyed.
- String startupMessage

  message to print at startup when proceeding to instantiate objects
- Graphics dakotaGraphics

  graphics and tabular data output handler used by meta-iterators, models, and approximations; encapsulated here so destroyed with the OutputManager
- unsigned short tabularFormat

  tabular format options; see enum
- int graphicsCntr

  used for x axis values in 2D graphics and for 1st column in tabular data
- std::ofstream tabularDataFStream

file stream for tabulation of graphics data within compute_response

- std::string tabularCntrLabel

  label for counter used in first line comment w/i the tabular data file

- std::string tabularInterfLabel

  label for interface used in first line comment w/i the tabular data file

- short outputLevel

  output level (for debugging only; not passed in)

- unsigned short resultsOutputFormat

  Output results format.

14.191.1 Detailed Description

Class to manage redirection of stdout/stderr, keep track of current redir state, and manage rank 0 output. Also manage tabular data output for post-processing with Matlab, Tecplot, etc. and delegate to Graphics for X Windows Graphics.

14.191.2 Constructor & Destructor Documentation

14.191.2.1 OutputManager (const ProgramOptions & *prog_opts*, int *dakota_world_rank* = 0, bool *dakota_mpirun_flag* = false)

Standard constructor, taking user-specified program options and optionally taking the rank of this process in Dakota's MPI_Comm.

Only get minimal information off ProgramOptions as may be updated later by broadcast.

References OutputManager::initial_redirects(), OutputManager::mpirunFlag, and Dakota::start_dakota_heartbeat().

14.191.3 Member Function Documentation

14.191.3.1 void pop_output_tag ( )

(Potentially) remove an output context and rebind streams

For now this assumes the tag is .<int>

References OutputManager::build_output_tag(), OutputManager::cerrRedirector, OutputManager::coutRedirector, OutputManager::fileTags, OutputManager::outputLevel, ConsoleRedirector::pop_back(), OutputManager::restart-Destinations, and OutputManager::worldRank.

Referenced by ParallelLibrary::pop_output_tag().

14.191.3.2 void open_tabular_datastream ( )

open the tabular datastream on iterator leaders

Opens the tabular data file stream and prints headings, one for each active continuous and discrete variable and one for each response function, using the variable and response function labels. This tabular data is used for post-processing of DAKOTA results in Matlab, Tecplot, etc.

References OutputManager::build_output_tag(), OutputManager::tabularDataFile, and OutputManager::tabular-DataFStream.

Referenced by NonHierarchSurrModel::create_tabular_datastream(), HierarchSurrModel::create_tabular_-datastream(), and Model::create_tabular_datastream().

14.191.3.3 void create_tabular_header (const Variables & *vars,* const Response & *response*)

output a complete header to the tabular datastream

Opens the tabular data file stream and prints headings, one for each active continuous and discrete variable and one for each response function, using the variable and response function labels. This tabular data is used for post-processing of DAKOTA results in Matlab, Tecplot, etc.

References OutputManager::tabularCntrLabel, OutputManager::tabularDataFStream, OutputManager::tabular-Format, and OutputManager::tabularInterfLabel.

Referenced by NonHierarchSurrModel::create_tabular_datastream(), HierarchSurrModel::create_tabular_-datastream(), and Model::create_tabular_datastream().

14.191.3.4 void add_tabular_data (const Variables & *vars,* const String & *iface,* const Response & *response*)

adds data to each window in the 2d graphics and adds a row to the tabular data file for the evaluation variables/response

Adds data to each 2d plot and each tabular data column (one for each active variable and for each response function). graphicsCntr is used for the x axis in the graphics and the first column in the tabular data.

References Response::active_set_request_vector(), Graphics::add_datapoint(), OutputManager::dakotaGraphics, OutputManager::graphicsCntr, OutputManager::tabularDataFStream, and OutputManager::tabularFormat.

Referenced by NonHierarchSurrModel::derived_auto_graphics(), HierarchSurrModel::derived_auto_graphics(), and Model::derived_auto_graphics().

The documentation for this class was generated from the following files:

- OutputManager.hpp
- OutputManager.cpp

14.192 OutputWriter Class Reference

Public Member Functions

- OutputWriter (std::ostream ∗output_stream)

  ostream constructor; used to construct a writer to existing stream, e.g., std::cout
- OutputWriter (const String &output_filename)

  file redirect constructor; opens an overwriting file stream to given name
- const String & filename () const

  the (possibly empty) file name for this stream
- std::ostream ∗ output_stream ()

  a pointer to the stream, either cout/cerr or a file

Protected Attributes

- String outputFilename

  the name of the output file (empty when constructed from pointer)
- std::ofstream outputFS

  file output stream for console text; only open if string non-empty
- std::ostream ∗ outputStream

  pointer to the stream for this writer

14.192.1 Detailed Description

Component to manage a redirected output or error stream

The documentation for this class was generated from the following files:

- OutputManager.hpp
- OutputManager.cpp

14.193 ParallelConfiguration Class Reference

Container class for a set of ParallelLevel list iterators that collectively identify a particular multilevel parallel configuration.

Public Member Functions

- ParallelConfiguration ()
  default constructor
- ParallelConfiguration (const ParallelConfiguration &pl)
  copy constructor
- ∼ParallelConfiguration ()
  destructor
- ParallelConfiguration & operator= (const ParallelConfiguration &pl)
  assignment operator
- const ParallelLevel & w_parallel_level () const
  return the ParallelLevel corresponding to miPLIters.front()
- const ParallelLevel & mi_parallel_level (size_t index=_NPOS) const
  return the ParallelLevel corresponding to miPLIters[index]
- const ParallelLevel & ie_parallel_level () const
  return the ParallelLevel corresponding to iePLIter
- const ParallelLevel & ea_parallel_level () const
  return the ParallelLevel corresponding to eaPLIter
- bool w_parallel_level_defined () const
  test for definition of world parallel level
- bool mi_parallel_level_defined (size_t index=_NPOS) const
  test for definition of meta-iterator-iterator parallel level
- bool ie_parallel_level_defined () const
  test for definition of iterator-evaluation parallel level
- bool ea_parallel_level_defined () const
  test for definition of evaluation-analysis parallel level
- ParLevLIter w_parallel_level_iterator () const
  return miPLIters.front()
- ParLevLIter mi_parallel_level_iterator (size_t index=_NPOS) const
  return miPLIters[index]
- ParLevLIter ie_parallel_level_iterator () const
  return iePLIter
- ParLevLIter ea_parallel_level_iterator () const
  return eaPLIter
- size_t mi_parallel_level_index (ParLevLIter pl_iter) const
  return the index within miPLIters corresponding to pl_iter
- size_t mi_parallel_level_last_index () const
  return the index of the last entry in miPLIters

Private Member Functions

- void assign (const ParallelConfiguration &pl)

    assign the attributes of the incoming pl to this object

Private Attributes

- short numParallelLevels

    number of parallel levels
- std::vector< ParLevLIter > miPLIters

    list iterator for world level followed by any concurrent iterator partitions (there may be multiple per parallel configuration instance)
- ParLevLIter iePLIter

    list iterator identifying the iterator-evaluation parallelLevel (there can only be one)
- ParLevLIter eaPLIter

    list iterator identifying the evaluation-analysis parallelLevel (there can only be one)
- ParLevLIter endPLIter

    snapshot of the end of ParallelLibrary::parallelLevels; used for detecting when a component of the parallel configuration has been initialized

Friends

- class ParallelLibrary

    the ParallelLibrary class has special access priveleges in order to streamline implementation

14.193.1 Detailed Description

Container class for a set of ParallelLevel list iterators that collectively identify a particular multilevel parallel configuration.

Rather than containing the multilevel parallel configuration directly, ParallelConfiguration instead provides a set of list iterators which point into a combined list of ParallelLevels. This approach allows different configurations to reuse ParallelLevels without copying them. A list of ParallelConfigurations is contained in ParallelLibrary (ParallelLibrary::parallelConfigurations).

14.193.2 Member Function Documentation

14.193.2.1 const ParallelLevel & mi_parallel_level (size_t *index* = _NPOS) const [inline]

return the ParallelLevel corresponding to miPLIters[index]

If a meaningful index is not provided, return the last mi parallel level. This is useful within the Model context, for which we need the lowest level partition after any meta-iterator recursions.

References ParallelConfiguration::miPLIters.

Referenced by ApplicationInterface::set_evaluation_communicators().

14.193.2.2 ParLevLIter mi_parallel_level_iterator (size_t *index* = _NPOS) const [inline]

return miPLIters[index]

If a meaningful index is not provided, return the last mi parallel level. This is useful within the Model context, for which we need the lowest level partition after any meta-iterator recursions.

References ParallelConfiguration::miPLIters.

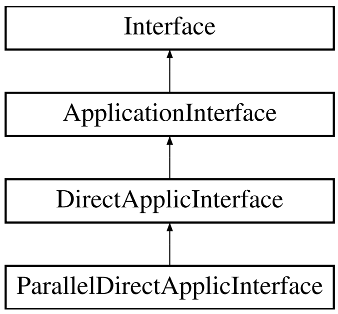
The documentation for this class was generated from the following file:

- ParallelLibrary.hpp

14.194 ParallelDirectApplicInterface Class Reference

Sample derived interface class for testing parallel simulator plug-ins using assign_rep().

Inheritance diagram for ParallelDirectApplicInterface:



Public Member Functions

- ParallelDirectApplicInterface (const Dakota::ProblemDescDB &problem_db, const MPI_Comm &analysis_-comm)

    constructor
- ∼ParallelDirectApplicInterface ()

    destructor

Protected Member Functions

- int derived_map_ac (const Dakota::String &ac_name)

    execute an analysis code portion of a direct evaluation invocation
- void derived_map_asynch (const Dakota::ParamResponsePair &pair)

    no-op hides base error; job batching occurs within wait_local_evaluations()
- void wait_local_evaluations (Dakota::PRPQueue &prp_queue)

    evaluate the batch of jobs contained in prp_queue
- void test_local_evaluations (Dakota::PRPQueue &prp_queue)

    invokes wait_local_evaluations() (no special nowait support)
- void set_communicators_checks (int max_eval_concurrency)

    no-op hides default run-time error checks at DirectApplicInterface level

Private Member Functions

- int text_book (const Dakota::RealVector &c_vars, const Dakota::ShortArray &asv, Dakota::RealVector &fn_-vals, Dakota::RealMatrix &fn_grads, Dakota::RealSymMatrixArray &fn_hessians)

    demo evaluator function for parallel plug-ins

Additional Inherited Members

14.194.1 Detailed Description

Sample derived interface class for testing parallel simulator plug-ins using assign_rep().

The plug-in ParallelDirectApplicInterface resides in namespace SIM and uses a copy of textbook() to perform parallel parameter to response mappings. It is used to demonstrate plugging in a parallel direct analysis driver into Dakota in library mode. Test input files can then use an analysis_driver of "plugin_textbook".

14.194.2 Member Function Documentation

14.194.2.1 void test_local_evaluations (Dakota::PRPQueue & *prp_queue*) [inline], [protected]

invokes wait_local_evaluations() (no special nowait support)

For use by ApplicationInterface::serve_evaluations_asynch(), which can provide a batch processing capability within message passing schedulers (called using chain ApplicationInterface::serve_evaluations() from Model::serve() from IteratorScheduler::run_iterator()).

References ParallelDirectApplicInterface::wait_local_evaluations().

The documentation for this class was generated from the following files:

- PluginParallelDirectApplicInterface.hpp
- PluginParallelDirectApplicInterface.cpp

14.195 ParallelLevel Class Reference

Container class for the data associated with a single level of communicator partitioning.

Public Member Functions

- ParallelLevel ()
  default constructor
- ParallelLevel (const ParallelLevel &pl)
  copy constructor
- ∼ParallelLevel ()
  destructor
- ParallelLevel & operator= (const ParallelLevel &pl)
  assignment operator
- bool dedicated_master () const
  return dedicatedMasterFlag
- bool server_master () const
  return serverMasterFlag
- bool message_pass () const
  return messagePass
- bool idle_partition () const
  return idlePartition
- int num_servers () const
  return numServers
- int processors_per_server () const
  return procsPerServer

- int processor_remainder () const

    return procRemainder
- const MPI_Comm & server_intra_communicator () const

    return serverIntraComm
- int server_communicator_rank () const

    return serverCommRank
- int server_communicator_size () const

    return serverCommSize
- const MPI_Comm & hub_server_intra_communicator () const

    return hubServerIntraComm
- int hub_server_communicator_rank () const

    return hubServerCommRank
- int hub_server_communicator_size () const

    return hubServerCommSize
- const MPI_Comm & hub_server_inter_communicator () const

    return hubServerInterComm
- MPI_Comm ∗ hub_server_inter_communicators () const

    return hubServerInterComms
- int server_id () const

    return serverId
- void read (MPIUnpackBuffer &s)

    read a ParallelLevel object from a packed MPI buffer
- void write (MPIPackBuffer &s) const

    write a ParallelLevel object to a packed MPI buffer
- bool null (const MPI_Comm &comm)

    test comm for MPI_COMM_NULL
- bool special (const MPI_Comm &comm)

    test comm for special identity that cannot be deallocated
- void clear ()

    deallocate the communicators in this ParallelLevel
- void alias (const ParallelLevel &pl)

    assign the attributes of the incoming pl to this object. For communicators, this is a lightweight copy which assigns the same pointer values as the incoming pl, resulting in the same context.
- void copy (const ParallelLevel &pl)

    deep copy the attributes of the incoming pl to this object using MPI_Comm_dup to create equivalent communicators with a unique context.
- void copy_config (const ParallelLevel &pl)

    copy the scalar attributes of the incoming pl to this object, omitting communicators

Private Attributes

- bool ownCommFlag

    signals Comm ownership for deallocation
- bool dedicatedMasterFlag

    signals dedicated master partitioning
- bool commSplitFlag

    signals a communicator split was used
- bool serverMasterFlag

    identifies master server processors
- bool messagePass

    flag for message passing at this level,
  < *indicating work assignment among servers*

- bool idlePartition

      identifies presence of an idle processor
  < *partition at this level*

- int numServers

  number of servers

- int procsPerServer

  processors per server

- int procRemainder

  proc remainder after equal distribution

- int serverId

  server identifier

- MPI_Comm serverIntraComm

  intracomm. for each server partition

- int serverCommRank

  rank in serverIntraComm

- int serverCommSize

  size of serverIntraComm

- MPI_Comm hubServerIntraComm

      intracomm for all serverCommRank==0
  < *w/i next higher level serverIntraComm*

- int hubServerCommRank

  rank in hubServerIntraComm

- int hubServerCommSize

  size of hubServerIntraComm

- MPI_Comm hubServerInterComm

      intercomm. between a server & the hub
  < *(on server partitions only)*

- MPI_Comm ∗ hubServerInterComms

  intercomm. array on hub processor

Friends

- class ParallelLibrary

  the ParallelLibrary class has special access priveleges in order to streamline implementation

14.195.1 Detailed Description

Container class for the data associated with a single level of communicator partitioning.

A list of these levels is contained in ParallelLibrary (ParallelLibrary::parallelLevels), which defines all of the parallelism levels across one or more multilevel parallelism configurations.

14.195.2 Member Function Documentation

14.195.2.1 void clear ( ) [inline]

deallocate the communicators in this ParallelLevel

This appears to be more robust outside of the destructor due to interactions among managed deallocation and default deallocation (e.g., explicitly freeing a communicator and then default deallocating its handle).

References ParallelLevel::dedicatedMasterFlag, ParallelLevel::hubServerInterComm, ParallelLevel::hubServerInterComms, ParallelLevel::hubServerIntraComm, ParallelLevel::idlePartition, ParallelLevel::numServers, ParallelLevel::ownCommFlag, ParallelLevel::serverId, ParallelLevel::serverIntraComm, and ParallelLevel::special().

The documentation for this class was generated from the following file:

- ParallelLibrary.hpp

14.196 ParallelLibrary Class Reference

Class for partitioning multiple levels of parallelism and managing message passing within these levels.

Public Member Functions

- ParallelLibrary ()

  default constructor (used for dummy_lib)
- ParallelLibrary (const MPIManager &mpi_mgr, ProgramOptions &prog_opts, OutputManager &output_mgr)

  stand-alone and default library mode constructor; don't require options
- ∼ParallelLibrary ()

  destructor
- const ParallelLevel & init_iterator_communicators (int iterator_servers, int procs_per_iterator, int min_procs_per_iterator, int max_procs_per_iterator, int max_iterator_concurrency, short default_config, short iterator_scheduling, bool peer_dynamic_avail)

  split MPI_COMM_WORLD into iterator communicators
- const ParallelLevel & init_evaluation_communicators (int evaluation_servers, int procs_per_evaluation, int min_procs_per_eval, int max_procs_per_eval, int max_evaluation_concurrency, int asynch_local_evaluation_concurrency, short default_config, short evaluation_scheduling, bool peer_dynamic_avail)

  split an iterator communicator into evaluation communicators
- const ParallelLevel & init_analysis_communicators (int analysis_servers, int procs_per_analysis, int min_procs_per_analysis, int max_procs_per_analysis, int max_analysis_concurrency, int asynch_local_analysis_concurrency, short default_config, short analysis_scheduling, bool peer_dynamic_avail)

  split an evaluation communicator into analysis communicators
- void print_configuration ()

  print the parallel level settings for a particular parallel configuration
- void push_output_tag (const ParallelLevel &pl)

  conditionally append an iterator server id tag to the hierarchical output tag, manage restart, and rebind cout/cerr
- void pop_output_tag (const ParallelLevel &pl)

  pop the last output tag and rebind streams as needed; pl isn't yet used, but may be in the future when we generalize to arbitrary output context switching
- void write_restart (const ParamResponsePair &prp)

  write a parameter/response set to the restart file
- ProgramOptions & program_options ()

  return programOptions reference
- OutputManager & output_manager ()

  return outputManager reference
- void terminate_modelcenter ()

  terminate ModelCenter if running
- void abort_helper (int code)

  finalize MPI with correct communicator for abort
- bool command_line_check () const

  return checkFlag
- bool command_line_pre_run () const

return preRunFlag
- bool command_line_run () const

  return runFlag
- bool command_line_post_run () const

  return postRunFlag
- bool command_line_user_modes () const

  return userModesFlag
- const String & command_line_pre_run_input () const

  preRunInput filename
- const String & command_line_pre_run_output () const

  preRunOutput filename
- const String & command_line_run_input () const

  runInput filename
- const String & command_line_run_output () const

  runOutput filename
- const String & command_line_post_run_input () const

  postRunInput filename
- const String & command_line_post_run_output () const

  postRunOutput fname
- void send (MPIPackBuffer &send_buff, int dest, int tag, const ParallelLevel &parent_pl, const ParallelLevel &child_pl)

  blocking buffer send at the current communication level
- void send (int &send_int, int dest, int tag, const ParallelLevel &parent_pl, const ParallelLevel &child_pl)

  blocking integer send at the current communication level
- void isend (MPIPackBuffer &send_buff, int dest, int tag, MPI_Request &send_req, const ParallelLevel &parent_pl, const ParallelLevel &child_pl)

  nonblocking buffer send at the current communication level
- void isend (int &send_int, int dest, int tag, MPI_Request &send_req, const ParallelLevel &parent_pl, const ParallelLevel &child_pl)

  nonblocking integer send at the current communication level
- void recv (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Status &status, const ParallelLevel &parent_pl, const ParallelLevel &child_pl)

  blocking buffer receive at the current communication level
- void recv (int &recv_int, int source, int tag, MPI_Status &status, const ParallelLevel &parent_pl, const ParallelLevel &child_pl)

  blocking integer receive at the current communication level
- void irecv (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Request &recv_req, const ParallelLevel &parent_pl, const ParallelLevel &child_pl)

  nonblocking buffer receive at the current communication level
- void irecv (int &recv_int, int source, int tag, MPI_Request &recv_req, const ParallelLevel &parent_pl, const ParallelLevel &child_pl)

  nonblocking integer receive at the current communication level
- void check_mi_index (size_t &index) const

  process _NPOS default and perform error checks
- void send_mi (int &send_int, int dest, int tag, size_t index=_NPOS)

  blocking send at the metaiterator-iterator communication level
- void isend_mi (int &send_int, int dest, int tag, MPI_Request &send_req, size_t index=_NPOS)

  nonblocking send at the metaiterator-iterator communication level
- void recv_mi (int &recv_int, int source, int tag, MPI_Status &status, size_t index=_NPOS)

  blocking receive at the metaiterator-iterator communication level
- void irecv_mi (int &recv_int, int source, int tag, MPI_Request &recv_req, size_t index=_NPOS)

  nonblocking receive at the metaiterator-iterator communication level

- void send_mi (MPIPackBuffer &send_buff, int dest, int tag, size_t index=_NPOS)

  blocking send at the metaiterator-iterator communication level
- void isend_mi (MPIPackBuffer &send_buff, int dest, int tag, MPI_Request &send_req, size_t index=_NPOS)

  nonblocking send at the metaiterator-iterator communication level
- void recv_mi (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Status &status, size_t index=_NPOS)

  blocking receive at the metaiterator-iterator communication level
- void irecv_mi (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Request &recv_req, size_t index=_NPOS)

  nonblocking receive at the metaiterator-iterator communication level
- void send_ie (int &send_int, int dest, int tag)

  blocking send at the iterator-evaluation communication level
- void isend_ie (int &send_int, int dest, int tag, MPI_Request &send_req)

  nonblocking send at the iterator-evaluation communication level
- void recv_ie (int &recv_int, int source, int tag, MPI_Status &status)

  blocking receive at the iterator-evaluation communication level
- void irecv_ie (int &recv_int, int source, int tag, MPI_Request &recv_req)

  nonblocking receive at the iterator-evaluation communication level
- void send_ie (MPIPackBuffer &send_buff, int dest, int tag)

  blocking send at the iterator-evaluation communication level
- void isend_ie (MPIPackBuffer &send_buff, int dest, int tag, MPI_Request &send_req)

  nonblocking send at the iterator-evaluation communication level
- void recv_ie (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Status &status)

  blocking receive at the iterator-evaluation communication level
- void irecv_ie (MPIUnpackBuffer &recv_buff, int source, int tag, MPI_Request &recv_req)

  nonblocking receive at the iterator-evaluation communication level
- void send_ea (int &send_int, int dest, int tag)

  blocking send at the evaluation-analysis communication level
- void isend_ea (int &send_int, int dest, int tag, MPI_Request &send_req)

  nonblocking send at the evaluation-analysis communication level
- void recv_ea (int &recv_int, int source, int tag, MPI_Status &status)

  blocking receive at the evaluation-analysis communication level
- void irecv_ea (int &recv_int, int source, int tag, MPI_Request &recv_req)

  nonblocking receive at the evaluation-analysis communication level
- void bcast (int &data, const ParallelLevel &pl)

  broadcast an integer across the serverIntraComm of a ParallelLevel
- void bcast (short &data, const ParallelLevel &pl)

  broadcast an integer across the serverIntraComm of a ParallelLevel
- void bcast (MPIPackBuffer &send_buff, const ParallelLevel &pl)

  broadcast a MPIPackBuffer across the serverIntraComm of a ParallelLevel
- void bcast (MPIUnpackBuffer &recv_buff, const ParallelLevel &pl)

  broadcast a MPIUnpackBuffer across the serverIntraComm of a ParallelLevel
- void bcast_hs (int &data, const ParallelLevel &pl)

  broadcast an integer across the hubServerIntraComm of a ParallelLevel
- void bcast_hs (MPIPackBuffer &send_buff, const ParallelLevel &pl)

  broadcast a MPIPackBuffer across the hubServerIntraComm of a ParallelLevel
- void bcast_hs (MPIUnpackBuffer &recv_buff, const ParallelLevel &pl)

  broadcast a MPIUnpackBuffer across the hubServerIntraComm of a ParallelLevel
- void bcast_w (int &data)

  broadcast an integer across MPI_COMM_WORLD
- void bcast_i (int &data, size_t index=_NPOS)

  broadcast an integer across an iterator communicator

- void bcast_i (short &data, size_t index=_NPOS)

  broadcast a short integer across an iterator communicator
- void bcast_e (int &data)

  broadcast an integer across an evaluation communicator
- void bcast_a (int &data)

  broadcast an integer across an analysis communicator
- void bcast_mi (int &data, size_t index=_NPOS)

  broadcast an integer across a metaiterator-iterator intra communicator
- void bcast_w (MPIPackBuffer &send_buff)

  broadcast a packed buffer across MPI_COMM_WORLD
- void bcast_i (MPIPackBuffer &send_buff, size_t index=_NPOS)

  broadcast a packed buffer across an iterator communicator
- void bcast_e (MPIPackBuffer &send_buff)

  broadcast a packed buffer across an evaluation communicator
- void bcast_a (MPIPackBuffer &send_buff)

  broadcast a packed buffer across an analysis communicator
- void bcast_mi (MPIPackBuffer &send_buff, size_t index=_NPOS)

  broadcast a packed buffer across a metaiterator-iterator intra communicator
- void bcast_w (MPIUnpackBuffer &recv_buff)

  matching receive for packed buffer broadcast across MPI_COMM_WORLD
- void bcast_i (MPIUnpackBuffer &recv_buff, size_t index=_NPOS)

  matching receive for packed buffer bcast across an iterator communicator
- void bcast_e (MPIUnpackBuffer &recv_buff)

  matching receive for packed buffer bcast across an evaluation communicator
- void bcast_a (MPIUnpackBuffer &recv_buff)

  matching receive for packed buffer bcast across an analysis communicator
- void bcast_mi (MPIUnpackBuffer &recv_buff, size_t index=_NPOS)

  matching recv for packed buffer bcast across a metaiterator-iterator intra comm
- void barrier_w ()

  enforce MPI_Barrier on MPI_COMM_WORLD
- void barrier_i (size_t index=_NPOS)

  enforce MPI_Barrier on an iterator communicator
- void barrier_e ()

  enforce MPI_Barrier on an evaluation communicator
- void barrier_a ()

  enforce MPI_Barrier on an analysis communicator
- void reduce_sum_ea (double ∗local_vals, double ∗sum_vals, int num_vals)

  compute a sum over an eval-analysis intra-communicator using MPI_Reduce
- void reduce_sum_a (double ∗local_vals, double ∗sum_vals, int num_vals)

  compute a sum over an analysis communicator using MPI_Reduce
- void test (MPI_Request &request, int &test_flag, MPI_Status &status)

  test a nonblocking send/receive request for completion
- void wait (MPI_Request &request, MPI_Status &status)

  wait for a nonblocking send/receive request to complete
- void waitall (int num_recvs, MPI_Request ∗&recv_reqs)

  wait for all messages from a series of nonblocking receives
- void waitsome (int num_sends, MPI_Request ∗&recv_requests, int &num_recvs, int ∗&index_array, MPI_-Status ∗&status_array)

  wait for at least one message from a series of nonblocking receives but complete all that are available
- void free (MPI_Request &request)

  free an MPI_Request

- int world_size () const

  return MPIManager::worldSize
- int world_rank () const

  return MPIManager::worldRank
- bool mpirun_flag () const

  return MPIManager::mpirunFlag
- bool is_null () const

  return dummyFlag
- Real parallel_time () const

  returns current MPI wall clock time
- void parallel_configuration_iterator (ParConfigLIter pc_iter)

  set the current ParallelConfiguration node
- ParConfigLIter parallel_configuration_iterator () const

  return the current ParallelConfiguration node
- const ParallelConfiguration & parallel_configuration () const

  return the current ParallelConfiguration instance
- size_t num_parallel_configurations () const

  returns the number of entries in parallelConfigurations
- bool parallel_configuration_is_complete ()

  identifies if the current ParallelConfiguration has been fully populated
- void increment_parallel_configuration (ParLevLIter mi_pl_iter)

  add a new node to parallelConfigurations and increment currPCIter; limit miPLIters within new configuration to mi_pl_iter level
- void increment_parallel_configuration ()

  add a new node to parallelConfigurations and increment currPCIter; copy all of miPLIters into new configuration
- bool w_parallel_level_defined () const

  test current parallel configuration for definition of world parallel level
- bool mi_parallel_level_defined (size_t index=_NPOS) const

  test current parallel configuration for definition of meta-iterator-iterator parallel level
- bool ie_parallel_level_defined () const

  test current parallel configuration for definition of iterator-evaluation parallel level
- bool ea_parallel_level_defined () const

  test current parallel configuration for definition of evaluation-analysis parallel level
- ParLevLIter w_parallel_level_iterator ()

  for this level, access through ParallelConfiguration is not necessary
- size_t parallel_level_index (ParLevLIter pl_iter)

  return the index within parallelLevels corresponding to pl_iter
- std::vector< MPI_Comm > analysis_intra_communicators ()

  return the set of analysis intra communicators for all parallel configurations (used for setting up direct simulation interfaces prior to execution time).

Private Member Functions

- void init_mpi_comm ()

  convenience function for initializing DAKOTA's top-level MPI communicators, based on dakotaMPIComm
- void initialize_timers ()

  initialize DAKOTA and UTILIB timers
- void output_timers ()

  conditionally output timers in destructor

- void init_communicators (const ParallelLevel &parent_pl, int num_servers, int procs_per_server, int min_procs_per_server, int max_procs_per_server, int max_concurrency, int asynch_local_concurrency, short default_config, short scheduling_override, bool peer_dynamic_avail)

    split a parent communicator into child server communicators
- void split_communicator_dedicated_master (const ParallelLevel &parent_pl, ParallelLevel &child_pl)

    split a parent communicator into a dedicated master processor and num_servers child communicators
- void split_communicator_peer_partition (const ParallelLevel &parent_pl, ParallelLevel &child_pl)

    split a parent communicator into num_servers peer child communicators (no dedicated master processor)
- void resolve_inputs (ParallelLevel &child_pl, int avail_procs, int min_procs_per_server, int max_procs_per_server, int max_concurrency, int capacity_multiplier, short default_config, short scheduling_override, bool peer_dynamic_avail, bool print_rank)

    resolve user inputs into a sensible partitioning scheme
- void bcast (int &data, const MPI_Comm &comm)

    broadcast an integer across a communicator
- void bcast (short &data, const MPI_Comm &comm)

    broadcast a short integer across a communicator
- void bcast (MPIPackBuffer &send_buff, const MPI_Comm &comm)

    send a packed buffer across a communicator using a broadcast
- void bcast (MPIUnpackBuffer &recv_buff, const MPI_Comm &comm)

    matching receive for a packed buffer broadcast
- void barrier (const MPI_Comm &comm)

    enforce MPI_Barrier on comm
- void reduce_sum (double ∗local_vals, double ∗sum_vals, int num_vals, const MPI_Comm &comm)

    compute a sum over comm using MPI_Reduce
- void check_error (const String &err_source, int err_code)

    check the MPI return code and abort if error
- void alias_as_server_comm (const ParallelLevel &parent_pl, ParallelLevel &child_pl)

    convenience function for updating child serverIntraComm from parent serverIntraComm (shallow Comm copy)
- void copy_as_server_comm (const ParallelLevel &parent_pl, ParallelLevel &child_pl)

    convenience function for updating child serverIntraComm from parent serverIntraComm (deep Comm copy)
- void alias_as_hub_server_comm (const ParallelLevel &parent_pl, ParallelLevel &child_pl)

    convenience function for updating child hubServerIntraComm from parent serverIntraComm (shallow Comm copy)
- void copy_as_hub_server_comm (const ParallelLevel &parent_pl, ParallelLevel &child_pl)

    convenience function for updating child hubServerIntraComm from parent serverIntraComm (deep Comm copy)

Private Attributes

- const MPIManager & mpiManager

    reference to the MPI manager with Dakota's MPI options
- ProgramOptions & programOptions

    programOptions is non-const due to updates from broadcast
- OutputManager & outputManager

    Non-const output handler to help with file redirection.
- bool dummyFlag

    prevents multiple MPI_Finalize calls due to dummy_lib
- bool outputTimings

    timing info only beyond help/version/check
- Real startCPUTime

    start reference for UTILIB CPU timer
- Real startWCTime

    start reference for UTILIB wall clock timer

- Real startMPITime

  start reference for MPI wall clock timer
- long startClock

  `start reference for local clock() timer measuring`
  < parent+child CPU
- std::list< ParallelLevel > parallelLevels

  the complete set of parallelism levels for managing multilevel parallelism among one or more configurations
- std::list< ParallelConfiguration > parallelConfigurations

  the set of parallel configurations which manage list iterators for indexing into parallelLevels
- ParConfigLIter currPCIter

  list iterator identifying the current node in parallelConfigurations

14.196.1 Detailed Description

Class for partitioning multiple levels of parallelism and managing message passing within these levels.

The ParallelLibrary class encapsulates all of the details of performing message passing within multiple levels of parallelism. It provides functions for partitioning of levels according to user configuration input and functions for passing messages within and across MPI communicators for each of the parallelism levels. If support for other message-passing libraries beyond MPI becomes needed (PVM, ...), then ParallelLibrary would be promoted to a base class with virtual functions to encapsulate the library-specific syntax.

14.196.2 Constructor & Destructor Documentation

14.196.2.1 ParallelLibrary ( )

default constructor (used for dummy_lib)

This constructor is used for creation of the global dummy_lib object, which is used to satisfy initialization requirements when the real ParallelLibrary object is not available.

14.196.2.2 ParallelLibrary (const MPIManager & *mpi_mgr*, ProgramOptions & *prog_opts*, OutputManager & *output_mgr*)

stand-alone and default library mode constructor; don't require options

library mode constructor accepting communicator

TODO: Update comment.

Same constructor is used for executable and library environments and sequencing of object construction is ordered, so no need to separately get updates off command line (programOptions)

References ParallelLibrary::init_mpi_comm(), and ParallelLibrary::initialize_timers().

14.196.3 Member Function Documentation

14.196.3.1 void push_output_tag (const ParallelLevel & *pl*)

conditionally append an iterator server id tag to the hierarchical output tag, manage restart, and rebind cout/cerr

If the user has specified the use of files for DAKOTA standard output and/or standard error, then bind these filenames to the Cout/Cerr macros. In addition, if concurrent iterators are to be used, create and tag multiple output streams in order to prevent jumbled output. Manage restart file(s) by processing any incoming evaluations from an old restart file and by setting up the binary output stream for new evaluations. Only master iterator processor(s) read & write restart information. This function must follow init_iterator_communicators so that restart can be managed properly for concurrent iterator strategies. In the case of concurrent iterators, each iterator has its own restart file tagged with iterator number.

References ParallelLibrary::bcast(), ParallelLevel::dedicatedMasterFlag, OutputManager::graph2DFlag, ParallelLevel::hubServerCommRank, ParallelLevel::hubServerCommSize, ParallelLevel::hubServerIntraComm, ParallelLevel::numServers, ParallelLibrary::outputManager, ParallelLibrary::programOptions, OutputManager::push_output_tag(), OutputManager::resultsOutputFile, OutputManager::resultsOutputFlag, ParallelLevel::serverCommRank, ParallelLevel::serverId, MPIPackBuffer::size(), OutputManager::tabularDataFile, and OutputManager::tabularDataFlag.

Referenced by Environment::construct(), and IteratorScheduler::partition().

14.196.3.2 void terminate_modelcenter ( )

terminate ModelCenter if running

Close streams associated with manage_outputs and manage_restart and terminate any additional services that may be active.

References Dakota::abort_handler(), Dakota::dc_ptr_int, and Dakota::mc_ptr_int.

Referenced by ParallelLibrary::∼ParallelLibrary().

14.196.3.3 void increment_parallel_configuration (ParLevLIter *mi_pl_iter*) [inline]

add a new node to parallelConfigurations and increment currPCIter; limit miPLIters within new configuration to mi_pl_iter level

Called from the ParallelLibrary ctor and from Model::init_communicators(). An increment is performed for each Model initialization except the first (which inherits the world level from the first partial configuration).

References ParallelLibrary::currPCIter, ParallelConfiguration::eaPLIter, ParallelConfiguration::endPLIter, ParallelConfiguration::iePLIter, ParallelConfiguration::miPLIters, ParallelConfiguration::numParallelLevels, ParallelLibrary::parallelConfigurations, and ParallelLibrary::parallelLevels.

Referenced by Iterator::init_communicators(), and Model::init_communicators().

14.196.3.4 void init_mpi_comm ( ) [private]

convenience function for initializing DAKOTA's top-level MPI communicators, based on dakotaMPIComm

shared function for initializing based on passed MPI_Comm

References Dakota::abort_handler(), MPIManager::dakota_mpi_comm(), ParallelLibrary::increment_parallel_configuration(), ParallelLibrary::mpiManager, MPIManager::mpirun_flag(), ParallelLevel::numServers, ParallelLibrary::outputManager, ParallelLibrary::parallelLevels, ParallelLevel::procsPerServer, ParallelLevel::serverCommRank, ParallelLevel::serverCommSize, ParallelLevel::serverId, ParallelLevel::serverIntraComm, ParallelLevel::serverMasterFlag, ParallelLibrary::startMPITime, OutputManager::startup_message(), MPIManager::world_rank(), and MPIManager::world_size().

Referenced by ParallelLibrary::ParallelLibrary().

14.196.3.5 void init_communicators (const ParallelLevel & *parent_pl*, int *num_servers*, int *procs_per_server*, int *min_procs_per_server*, int *max_procs_per_server*, int *max_concurrency*, int *asynch_local_concurrency*, short *default_config*, short *scheduling_override*, bool *peer_dynamic_avail*) [private]

split a parent communicator into child server communicators

Split parent communicator into concurrent child server partitions as specified by the passed parameters. This constructs new child intra-communicators and parent-child inter-communicators. This fn is called from MetaIterators and NestedModel for the concurrent iterator level and from ApplicationInterface::init_communicators() for the concurrent evaluation and concurrent analysis levels.

References ParallelLibrary::currPCIter, ParallelLevel::dedicatedMasterFlag, ParallelLevel::messagePass, ParallelLevel::numServers, ParallelLibrary::parallelLevels, ParallelLevel::procsPerServer, ParallelLibrary::resolve_inputs(), ParallelLevel::serverCommRank, ParallelLevel::serverCommSize, ParallelLibrary::split_communicator_dedicated_master(), and ParallelLibrary::split_communicator_peer_partition().

Referenced by ParallelLibrary::init_analysis_communicators(), ParallelLibrary::init_evaluation_communicators(), and ParallelLibrary::init_iterator_communicators().

14.196.3.6 void resolve_inputs (**ParallelLevel** & *child_pl,* int *avail_procs,* int *min_procs_per_server,* int *max_procs_per_server,* int *max_concurrency,* int *capacity_multiplier,* short *default_config,* short *scheduling_override,* bool *peer_dynamic_avail,* bool *print_rank*) [private]

resolve user inputs into a sensible partitioning scheme

This function is responsible for the "auto-configure" intelligence of DAKOTA. It resolves a variety of inputs and overrides into a sensible partitioning configuration for a particular parallelism level. It also handles the general case in which a user's specification request does not divide out evenly with the number of available processors for the level. If num_servers & procs_per_server are both nondefault, then the former takes precedence.

References Dakota::abort_handler(), ParallelLevel::dedicatedMasterFlag, ParallelLevel::numServers, ParallelLevel::procRemainder, and ParallelLevel::procsPerServer.

Referenced by ParallelLibrary::init_communicators().

The documentation for this class was generated from the following files:

- ParallelLibrary.hpp
- ParallelLibrary.cpp

14.197 ParamResponsePair Class Reference

Container class for a variables object, a response object, and an evaluation id.

Public Member Functions

- ParamResponsePair ()
  default constructor
- ParamResponsePair (const Variables &vars, const String &interface_id, const Response &response, bool deep_copy=false)
  alternate constructor for temporaries
- ParamResponsePair (const Variables &vars, const String &interface_id, const Response &response, const int eval_id, bool deep_copy=true)
  standard constructor for history uses
- ParamResponsePair (const ParamResponsePair &pair)
  copy constructor
- ∼ParamResponsePair ()
  destructor
- ParamResponsePair & operator= (const ParamResponsePair &pair)
  assignment operator
- void read (std::istream &s)
  read a ParamResponsePair object from an std::istream
- void write (std::ostream &s) const
  write a ParamResponsePair object to an std::ostream
- void read_annotated (std::istream &s)
  read a ParamResponsePair object in annotated format from an std::istream

- void write_annotated (std::ostream &s) const
  write a ParamResponsePair object in annotated format to an std::ostream
- void write_tabular (std::ostream &s, unsigned short tabular_format) const
  write a ParamResponsePair object in tabular format (all variables active/inactive) to an std::ostream
- void write_tabular_labels (std::ostream &s, unsigned short tabular_format) const
  write PRP labels in tabular format to an std::ostream
- void read (MPIUnpackBuffer &s)
  read a ParamResponsePair object from a packed MPI buffer
- void write (MPIPackBuffer &s) const
  write a ParamResponsePair object to a packed MPI buffer
- int eval_id () const
  return the evaluation identifier
- void eval_id (int id)
  set the evaluation identifier
- const String & interface_id () const
  return the interface identifier from evalInterfaceIds
- void interface_id (const String &id)
  set the interface identifier within evalInterfaceIds
- const IntStringPair & eval_interface_ids () const
  return the aggregate eval/interface identifier from the response object
- const Variables & variables () const
  return the parameters object
- Variables & variables ()
  return the parameters object
- void variables (const Variables &vars)
  set the parameters object
- const Response & response () const
  return the response object
- Response & response ()
  return the response object
- void response (const Response &resp)
  set the response object
- IntResponsePair response_pair () const
  return evaluation id and response as a std::pair
- const ActiveSet & active_set () const
  return the active set object from the response object
- void active_set (const ActiveSet &set)
  set the active set object within the response object

Private Member Functions

- template<class Archive >
  void serialize (Archive &ar, const unsigned int version)
  serialize the PRP: write and read are symmetric for this class

Private Attributes

- Variables prpVariables
  the set of parameters for the function evaluation
- Response prpResponse
  the response set for the function evaluation
- IntStringPair evalInterfaceIds
  the evalInterfaceIds aggregate

Friends

- class boost::serialization::access

  allow boost access to serialize this class
- bool operator== (const ParamResponsePair &pair1, const ParamResponsePair &pair2)

  equality operator
- bool operator!= (const ParamResponsePair &pair1, const ParamResponsePair &pair2)

  inequality operator

14.197.1 Detailed Description

Container class for a variables object, a response object, and an evaluation id.

ParamResponsePair provides a container class for association of the input for a particular function evaluation (a variables object) with the output from this function evaluation (a response object), along with an evaluation identifier. This container defines the basic unit used in the data_pairs cache, in restart file operations, and in a variety of scheduling algorithm queues. With the advent of STL, replacement of arrays of this class with map<> and pair<> template constructs may be possible (using map<pair<int,String>, pair<Variables,Response> >, for example), assuming that deep copies, I/O, alternate constructors, etc., can be adequately addressed. Boost tuple<> may also be a candidate.

14.197.2 Constructor & Destructor Documentation

14.197.2.1 ParamResponsePair (const Variables & *vars*, const String & *interface_id*, const Response & *response*, bool *deep_copy* = false) [inline]

alternate constructor for temporaries

Uses of this constructor often employ the standard Variables and Response copy constructors to share representations since this constructor is commonly used for search_pairs (which are local instantiations that go out of scope prior to any changes to values; i.e., they are not used for history).

14.197.2.2 ParamResponsePair (const Variables & *vars*, const String & *interface_id*, const Response & *response*, const int *eval_id*, bool *deep_copy* = true) [inline]

standard constructor for history uses

Uses of this constructor often do not share representations since deep copies are used when history mechanisms (e.g., data_pairs and beforeSynchCorePRPQueue) are involved.

14.197.3 Member Function Documentation

14.197.3.1 void read (MPIUnpackBuffer & *s*) [inline]

read a ParamResponsePair object from a packed MPI buffer

interfaceId is omitted since master processor retains interface ids and communicates asv and response data only with slaves.

References ParamResponsePair::evalInterfaceIds, ParamResponsePair::prpResponse, and ParamResponsePair::prpVariables.

14.197.3.2 void write (MPIPackBuffer & *s*) const [inline]

write a ParamResponsePair object to a packed MPI buffer interfaceId is omitted since master processor retains interface ids and communicates asv and response data only with slaves.

References ParamResponsePair::evalInterfaceIds, ParamResponsePair::prpResponse, and ParamResponsePair::prpVariables.

14.197.4 Member Data Documentation

14.197.4.1 IntStringPair evalInterfaceIds [private]

the evalInterfaceIds aggregate

the function evaluation identifier (assigned from Interface::evalIdCntr) is paired with the interface used to generate the response object. Used in PRPCache id_vars_set_compare to prevent duplicate detection on results from different interfaces. evalInterfaceIds belongs here rather than in Response since some Response objects involve consolidation of several fn evals (e.g., Model::synchronize_derivatives()) that are not, in total, generated by a single interface. The prPair, on the other hand, is used for storage of all low level fn evals that get evaluated in ApplicationInterface::map().

Referenced by ParamResponsePair::eval_id(), ParamResponsePair::eval_interface_ids(), ParamResponsePair::interface_id(), ParamResponsePair::operator=(), Dakota::operator==(), ParamResponsePair::read(), ParamResponsePair::response_pair(), and ParamResponsePair::write().

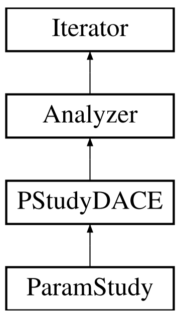
The documentation for this class was generated from the following file:

- ParamResponsePair.hpp

14.198 ParamStudy Class Reference

Class for vector, list, centered, and multidimensional parameter studies.

Inheritance diagram for ParamStudy:



Public Member Functions

- ParamStudy (ProblemDescDB &problem_db, Model &model)

  constructor
- ∼ParamStudy ()

  destructor
- bool resize ()

  reinitializes iterator based on new variable size
- void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

- void post_input ()

  read tabular data for post-run mode
- void post_run (std::ostream &s)

  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- void archive_model_variables (const Model &, size_t idx) const override

  Archive variables for parameter set idx.
- void archive_model_response (const Response &, size_t idx) const override

  Archive responses for parameter set idx.

Protected Member Functions

- void archive_allocate_sets () const

  Allocate space to archive parameters and responses.

Private Member Functions

- void sample ()

  performs the parameter study by sampling from a list of points
- void vector_loop ()

  performs the parameter study by sampling along a vector, starting from an initial point followed by numSteps increments along continous/discrete step vectors
- void centered_loop ()

  performs a number of plus and minus offsets for each parameter centered about an initial point
- void multidim_loop ()

  performs a full factorial combination for all intersections defined by a set of multidimensional partitions
- bool load_distribute_points (const String &points_filename, unsigned short tabular_format, bool active_only)

  load list of points from data file and distribute among listCVPoints, listDIVPoints, listDSVPoints, and listDRVPoints
- template< typename OrdinalType , typename ScalarTypeA , typename ScalarTypeC , typename ScalarTypeDI , typename ScalarTypeDS , typename ScalarTypeDR >
  bool distribute (const Teuchos::SerialDenseVector< OrdinalType, ScalarTypeA > &all_data, Teuchos::SerialDenseVector< OrdinalType, ScalarTypeC > &c_data, Teuchos::SerialDenseVector< OrdinalType, ScalarTypeDI > &di_data, Teuchos::SerialDenseVector< OrdinalType, ScalarTypeDS > &ds_data, Teuchos::SerialDenseVector< OrdinalType, ScalarTypeDR > &dr_data)

  distributes incoming all vector in standard variable ordering among continuous, discrete int, discrete string, and discrete real vectors
- template< typename ScalarType >
  bool distribute (const std::vector< ScalarType > &all_data, std::vector< ScalarType > &c_data, std::vector< ScalarType > &di_data, std::vector< ScalarType > &ds_data, std::vector< ScalarType > &dr_data)

  distributes incoming all array in standard variable ordering among continuous, discrete int, discrete string, and discrete real arrays
- bool distribute_list_of_points (const RealVector &list_of_pts)

  distributes list_of_pts coming from user spec among listCVPoints, listDIVPoints, listDSVPoints, and listDRVPoints
- void final_point_to_step_vector ()

  compute step vectors from finalPoint, initial points, and numSteps
- void distribute_partitions ()

  compute step vectors from {cont,discInt,discString,discReal}VarPartitions and global bounds
- bool check_num_steps (int num_steps)

  perform error checks on numSteps
- bool check_step_vector (const RealVector &step_vector)

  perform error checks on numSteps

- bool check_final_point (const RealVector &final_pt)

  perform error checks on finalPoint
- bool check_steps_per_variable (const IntVector &steps_per_var)

  perform error checks on stepsPerVariable
- bool check_variable_partitions (const UShortArray &partitions)

  perform error checks on variable partitions
- bool check_finite_bounds ()

  check for finite variable bounds within iteratedModel, as required for computing partitions of finite ranges
- bool check_ranges_sets (int num_steps)

  sanity check for vector parameter study
- bool check_ranges_sets (const IntVector &c_steps, const IntVector &di_steps, const IntVector &ds_steps, const IntVector &dr_steps)

  sanity check for centered parameter study
- bool check_sets (const IntVector &c_steps, const IntVector &di_steps, const IntVector &ds_steps, const Int-Vector &dr_steps)

  sanity check for increments along int/real set dimensions
- int integer_step (int range, int num_steps) const

  check for integer remainder and return step
- int index_step (size_t start, size_t end, int num_steps) const

  check for out of bounds and index remainder and return step
- void c_step (size_t c_index, int increment, Variables &vars)

  helper function for performing a continuous step in one variable
- void dri_step (size_t di_index, int increment, Variables &vars)

  helper function for performing a discrete step in an integer range variable
- void dsi_step (size_t di_index, int increment, const IntSet &values, Variables &vars)

  helper function for performing a discrete step in an integer set variable
- void dss_step (size_t ds_index, int increment, const StringSet &values, Variables &vars)

  helper function for performing a discrete step in an string set variable
- void dsr_step (size_t dr_index, int increment, const RealSet &values, Variables &vars)

  helper function for performing a discrete step in a real set variable
- void reset (Variables &vars)

  reset vars to initial point (center)
- void centered_header (const String &type, size_t var_index, int step, size_t hdr_index)

  store a centered parameter study header within allHeaders
- void archive_allocate_cps () const

  specialized per-variable slice output for centered param study
- void archive_cps_vars (const Model &model, size_t idx) const

  specialized per-variable slice output for centered param study
- void archive_cps_resp (const Response &response, size_t idx) const

  specialized per-variable slice output for centered param study
- void index_to_var_step (const size_t study_idx, size_t &var_idx, size_t &step_idx) const

  map an overall parameter study (zero-based) evaluation index to the (zero-based) variable index (among all variables) and the (zero-based) step index within that variable

Private Attributes

- size_t numEvals

  total number of parameter study evaluations computed from specification
- RealVectorArray listCVPoints

  array of continuous evaluation points for the list_parameter_study
- IntVectorArray listDIVPoints

array of discrete int evaluation points for the list_parameter_study

- StringMulti2DArray listDSVPoints

  array of discrete string evaluation points for the list_parameter_study
- RealVectorArray listDRVPoints

  array of discrete real evaluation points for the list_parameter_study
- RealVector initialCVPoint

  the continuous start point for vector and centered parameter studies
- IntVector initialDIVPoint

  the discrete int start point for vector and centered parameter studies
- StringMultiArray initialDSVPoint

  the discrete string start point for vector and centered parameter studies
- RealVector initialDRVPoint

  the discrete real start point for vector and centered parameter studies
- RealVector finalCVPoint

  the continuous ending point for vector_parameter_study
- IntVector finalDIVPoint

  the discrete int range value or set index ending point for vector_parameter_study
- IntVector finalDSVPoint

  the discrete string set index ending point for vector_parameter_study
- IntVector finalDRVPoint

  the discrete real set index ending point for vector_parameter_study
- RealVector contStepVector

  the n-dimensional continuous increment
- IntVector discIntStepVector

  the n-dimensional discrete integer range value or set index increment
- IntVector discStringStepVector

  the n-dimensional discrete string set index increment
- IntVector discRealStepVector

  the n-dimensional discrete real set index increment
- int numSteps

  the number of times continuous/discrete step vectors are applied for vector_parameter_study (a specification option)
- IntVector stepsPerVariable

  number of offsets in the plus and the minus direction for each variable in a centered_parameter_study
- IntVector contStepsPerVariable

  number of offsets in the plus and the minus direction for each continuous variable in a centered_parameter_study
- IntVector discIntStepsPerVariable

  number of offsets in the plus and the minus direction for each discrete integer variable in a centered_parameter_study
- IntVector discStringStepsPerVariable

  number of offsets in the plus and the minus direction for each discrete string variable in a centered_parameter_study
- IntVector discRealStepsPerVariable

  number of offsets in the plus and the minus direction for each discrete real variable in a centered_parameter_study
- UShortArray contVarPartitions

  number of partitions for each continuous variable in a multidim_parameter_study
- UShortArray discIntVarPartitions

  number of partitions for each discrete integer variable in a multidim_parameter_study
- UShortArray discStringVarPartitions

  number of partitions for each discrete string variable in a multidim_parameter_study
- UShortArray discRealVarPartitions

  number of partitions for each discrete real variable in a multidim_parameter_study

Additional Inherited Members

14.198.1 Detailed Description

Class for vector, list, centered, and multidimensional parameter studies.

The ParamStudy class contains several algorithms for performing parameter studies of different types. The vector parameter study steps along an n-dimensional vector from an arbitrary initial point to an arbitrary final point in a specified number of steps. The centered parameter study performs a number of plus and minus offsets in each coordinate direction around a center point. A multidimensional parameter study fills an n-dimensional hypercube based on bounds and a specified number of partitions for each dimension. And the list parameter study provides for a user specification of a list of points to evaluate, which allows general parameter investigations not fitting the structure of vector, centered, or multidim parameter studies.

14.198.2 Member Function Documentation

14.198.2.1 void pre_run ( ) [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

References Dakota::abort_handler(), SharedVariablesData::active_components_totals(), Analyzer::allHeaders, Analyzer::allVariables, ParamStudy::centered_loop(), Variables::continuous_variables(), ParamStudy::contSteps-PerVariable, ParamStudy::contStepVector, ParamStudy::contVarPartitions, Variables::copy(), Dakota::copy_data(), Model::current_variables(), ParamStudy::discIntStepsPerVariable, ParamStudy::discIntStepVector, ParamStudy-::discIntVarPartitions, ParamStudy::discRealStepsPerVariable, ParamStudy::discRealStepVector, ParamStudy-::discRealVarPartitions, Variables::discrete_int_variables(), Variables::discrete_real_variables(), Variables::discrete-_string_variables(), ParamStudy::discStringStepsPerVariable, ParamStudy::discStringStepVector, ParamStudy-::discStringVarPartitions, ParamStudy::distribute_partitions(), ParamStudy::final_point_to_step_vector(), Param-Study::finalCVPoint, ParamStudy::finalDIVPoint, ParamStudy::finalDRVPoint, ParamStudy::finalDSVPoint, Param-Study::initialCVPoint, ParamStudy::initialDIVPoint, ParamStudy::initialDRVPoint, ParamStudy::initialDSVPoint, Iterator::iteratedModel, Iterator::method_enum_to_string(), Iterator::methodName, ParamStudy::multidim_loop(), Analyzer::numDiscreteStringVars, ParamStudy::numEvals, ParamStudy::numSteps, Iterator::outputLevel, Analyzer-::pre_run(), ParamStudy::sample(), Variables::shared_data(), Dakota::svd(), ParamStudy::vector_loop(), and Dakota::write_ordered().

14.198.2.2 void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References ParamStudy::archive_allocate_sets(), Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, Iterator::methodName, Analyzer::numLSqTerms, Analyzer::numObjFns, and Iterator::subIteratorFlag.

14.198.2.3 void post_run (std::ostream & *s*) [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Analyzer.

References ResultsManager::active(), Analyzer::allResponses, Analyzer::allVariables, SensAnalysisGlobal::archive_correlations(), SensAnalysisGlobal::compute_correlations(), Model::continuous_variable_labels(), Model::discrete_int_variable_labels(), Model::discrete_real_variable_labels(), Model::discrete_set_string_values(), Model::discrete_string_variable_labels(), Iterator::iteratedModel, Iterator::methodName, Analyzer::post_run(), PStudyDACE::pStudyDACESensGlobal, Model::response_labels(), Iterator::resultsDB, Iterator::run_identifier(), and Iterator::subIteratorFlag.

14.198.2.4 bool load_distribute_points (const String & *points_filename,* unsigned short *tabular_format,* bool *active_only*) [private]

load list of points from data file and distribute among listCVPoints, listDIVPoints, listDSVPoints, and listDRVPoints

Load from file and distribute points; using this function to manage construction of the temporary arrays. Historically all data was read as a real (mixture of values and indices), but now points_file is valued-based (reals, integers, strings) so file input matches tabular data output. Return false on success.

References Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Variables::copy(), Model::current_variables(), Model::discrete_int_lower_bounds(), Model::discrete_int_sets(), Model::discrete_int_upper_bounds(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Iterator::iteratedModel, ParamStudy::listCVPoints, ParamStudy::listDIVPoints, ParamStudy::listDRVPoints, ParamStudy::listDSVPoints, Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, ParamStudy::numEvals, and Dakota::set_value_to_index().

Referenced by ParamStudy::ParamStudy().

14.198.2.5 bool distribute_list_of_points (const RealVector & *list_of_pts*) [private]

distributes list_of_pts coming from user spec among listCVPoints, listDIVPoints, listDSVPoints, and listDRVPoints

Parse list of points into typed data containers; list_of_pts will contain values for continuous and discrete integer range, but indices for all discrete set types (int, string, real)

References Dakota::abort_handler(), Model::discrete_int_sets(), Model::discrete_int_variable_labels(), Model::discrete_real_variable_labels(), Model::discrete_set_int_values(), Model::discrete_set_real_values(), Model::discrete_set_string_values(), Model::discrete_string_variable_labels(), ParamStudy::distribute(), Iterator::iteratedModel, ParamStudy::listCVPoints, ParamStudy::listDIVPoints, ParamStudy::listDRVPoints, ParamStudy::listDSVPoints, Iterator::method_id(), Analyzer::numContinuousVars, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, ParamStudy::numEvals, and Dakota::set_index_to_value().

Referenced by ParamStudy::ParamStudy().

14.198.3 Member Data Documentation

14.198.3.1 IntVector stepsPerVariable [private]

number of offsets in the plus and the minus direction for each variable in a centered_parameter_study

The per-type step arrays below could be made views into this, instead of duplicating, but if so, distribute() will not be allowed to resize the individual vectors.

Referenced by ParamStudy::check_steps_per_variable(), and ParamStudy::index_to_var_step().

The documentation for this class was generated from the following files:

- ParamStudy.hpp
- ParamStudy.cpp

14.199 partial_prp_equality Struct Reference

predicate for comparing ONLY the interfaceId and Vars attributes of PRPair

Public Member Functions

- bool operator() (const ParamResponsePair &database_pr, const ParamResponsePair &search_pr) const
  access operator

14.199.1 Detailed Description

predicate for comparing ONLY the interfaceId and Vars attributes of PRPair

The documentation for this struct was generated from the following file:

- PRPMultiIndex.hpp

14.200 partial_prp_hash Struct Reference

wrapper to delegate to the ParamResponsePair hash_value function

Public Member Functions

- std::size_t operator() (const ParamResponsePair &prp) const
  access operator

14.200.1 Detailed Description

wrapper to delegate to the ParamResponsePair hash_value function

The documentation for this struct was generated from the following file:

- PRPMultiIndex.hpp

14.201 PebbldBranching Class Reference

Main Branching class for the PEBBL-based Minimizer.

Inherits branching.

Public Member Functions

- PebbldBranching ()
  Default Constructor.
- ∼PebbldBranching ()
  Destructor.
- pebbl::branchSub ∗ blankSub ()
  Method that returns an empty Sub-Branch.
- void **setModel** (Model &model)
- void **setIterator** (Iterator &iterator)

Protected Attributes

- Model parentModel

  Original model, before branching.
- Iterator nlpSolver

  Solver to be used at root node.
- RealVector cont_vars

  Initial variable values for root node.
- RealVector lower_bounds

  Lower bounds for root node.
- RealVector upper_bounds

  Upper bounds for root node.

Friends

- class **PebbldBranchSub**

14.201.1 Detailed Description

Main Branching class for the PEBBL-based Minimizer.

The documentation for this class was generated from the following files:

- PEBBLBranching.hpp
- PEBBLBranching.cpp

14.202 PebbldBranchSub Class Reference

Sub Branch class for the PEBBL-based Minimizer.

Inherits branchSub.

Public Member Functions

- PebbldBranchSub ()

  Constructor.
- ∼PebbldBranchSub ()

  Destructor.
- PebbldBranching ∗ global () const

  Returns a reference to the corresponding main Branching object.
- pebbl::branching ∗ bGlobal () const

  Returns a reference to the corresponding main Branching object.
- void setGlobalInfo (PebbldBranching ∗global_)

  Method that sets up the main Branching object.
- void setRootComputation ()

  Method that is called when declaring the current node as a root node.
- void boundComputation (double ∗controlParam)

  Method that does the Bounding Operation. In other words, it calls the optimization algorithm on the relaxed domain.
- bool candidateSolution ()

  Method called after the bounding operation, returns true if the bounding resulted in a possible solution to the original non-relaxed problem.

- pebbl::solution * extractSolution ()

  Method that returns a PEBBL-based solution.

- int splitComputation ()

  Method that determines how many branches are created and how. Returns the number of branches created from this object.

- pebbl::branchSub * makeChild (int whichChild)

  Method that returns a new PebbldBranchSub object based on Objective Function improvements and the number of branches.

- void pebbldSubAsChildOf (PebbldBranchSub *parent, int splitVar, int whichChild, std::vector< double > _candidate_x, RealVector _lower_bounds, RealVector _upper_bounds)

  Method that creates a new PebbldBranching object.

Protected Attributes

- PebbldBranching * globalPtr

  Pointer referring to all info passed to subproblem.

- Model subModel

  Model used for sub-problem.

- Iterator subNLPSolver

  Solver used for sub-problems.

- std::vector< double > candidate_x

  Candidate solution after solving sub-problem (also the bound)

- double candidate_objFn

  Objective value at the candidate solution.

- int splitVar

  Variable to branch on.

- RealVector cont_vars

  Initial variable values for sub-problem.

- RealVector lower_bounds

  Lower bounds for sub-problem.

- RealVector upper_bounds

  Upper bounds for sub-problem.

Friends

- class **PebbldBranching**

14.202.1 Detailed Description

Sub Branch class for the PEBBL-based Minimizer.

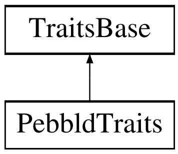
The documentation for this class was generated from the following files:

- PEBBLBranching.hpp
- PEBBLBranching.cpp

14.203 PebbldTraits Class Reference

Wrapper class for experimental PebbldMinimizer.

Inheritance diagram for PebbldTraits:



Public Member Functions

- PebbldTraits ()

    default constructor
- virtual ∼PebbldTraits ()

    destructor
- virtual bool is_derived ()

    A temporary query used in the refactor.
- bool supports_continuous_variables ()

    Return the flag indicating whether method supports continuous variables.
- bool supports_discrete_variables ()

    Return the flag indicating whether method supports discrete variables.
- bool supports_nonlinear_equality ()

    Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

    Return the flag indicating whether method supports nonlinear inequalities.

14.203.1 Detailed Description

Wrapper class for experimental PebbldMinimizer.

A version of TraitsBase specialized for Pebbld mptimizers

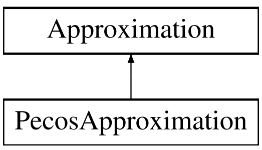
The documentation for this class was generated from the following file:

- PEBBLMinimizer.hpp

14.204 PecosApproximation Class Reference

Derived approximation class for global basis polynomials.

Inheritance diagram for PecosApproximation:



Public Member Functions

- PecosApproximation ()

  default constructor
- PecosApproximation (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

  standard ProblemDescDB-driven constructor
- PecosApproximation (const SharedApproxData &shared_data)

  alternate constructor
- ∼PecosApproximation ()

  destructor
- void expansion_coefficient_flag (bool coeff_flag)

  set pecosBasisApprox.configOptions.expansionCoeffFlag
- bool expansion_coefficient_flag () const

  get pecosBasisApprox.configOptions.expansionCoeffFlag
- void expansion_gradient_flag (bool grad_flag)

  set pecosBasisApprox.configOptions.expansionGradFlag
- bool expansion_gradient_flag () const

  get pecosBasisApprox.configOptions.expansionGradFlag
- void clear_component_effects ()

  clear unused Sobol' indices
- void compute_component_effects ()

  Performs global sensitivity analysis using Sobol' indices by computing component (main and interaction) effects.
- void compute_total_effects ()

  Performs global sensitivity analysis using Sobol' indices by computing total effects.
- const Pecos::RealVector & sobol_indices () const

  return polyApproxRep->sobolIndices
- const Pecos::RealVector & total_sobol_indices () const

  return polyApproxRep->totalSobolIndices
- size_t sparsity () const

  return the number of non-zero coefficients for this QoI
- Pecos::ULongULongMap sparse_sobol_index_map () const

  return RegressOrthogPolyApproximation::sparseSobolIndexMap
- const Pecos::RealVector & dimension_decay_rates () const

  return OrthogPolyApproximation::decayRates
- void allocate_arrays ()

  invoke Pecos::PolynomialApproximation::allocate_arrays()
- void initialize_covariance (Approximation &approx_2)

  initialize covariance accumulators with pointers to other QoI
- void clear_covariance_pointers ()

  clear covariance pointers to other QoI
- void initialize_products ()

  initialize covariance accumulators (also reinitialize after change in stats type)
- bool product_interpolants ()

  query whether product interpolants are defined (non-empty)
- Real mean ()

  return the mean of the expansion, where all active variables are random
- Real mean (const Pecos::RealVector &x)

  return the mean of the expansion for a given parameter vector, where a subset of the active variables are random
- Real combined_mean ()

  return the mean of the combined expansion, treating all variables as random

- Real combined_mean (const Pecos::RealVector &x)

  return the mean of the combined expansion for a given parameter vector, where a subset of the active variables are treated as random
- const Pecos::RealVector & mean_gradient ()

  return the gradient of the expansion mean for a given parameter vector, where all active variables are random
- const Pecos::RealVector & mean_gradient (const Pecos::RealVector &x, const Pecos::SizetArray &dvv)

  return the gradient of the expansion mean for a given parameter vector and given DVV, where a subset of the active variables are random
- Real variance ()

  return the variance of the expansion, where all active vars are random
- Real variance (const Pecos::RealVector &x)

  return the variance of the expansion for a given parameter vector, where a subset of the active variables are random
- const Pecos::RealVector & variance_gradient ()

  return the gradient of the expansion variance for a given parameter vector, where all active variables are random
- const Pecos::RealVector & variance_gradient (const Pecos::RealVector &x, const Pecos::SizetArray &dvv)

  return the gradient of the expansion variance for a given parameter vector and given DVV, where a subset of the active variables are random
- Real covariance (Approximation &approx_2)

  return the covariance between two response expansions, treating all variables as random
- Real covariance (const Pecos::RealVector &x, Approximation &approx_2)

  return the covariance between two response expansions, treating a subset of the variables as random
- Real combined_covariance (Approximation &approx_2)

  return the covariance between two combined response expansions, where all active variables are random
- Real combined_covariance (const Pecos::RealVector &x, Approximation &approx_2)

  return the covariance between two combined response expansions, where a subset of the active variables are random
- Real beta (bool cdf_flag, Real z_bar)

  return the reliability index (mapped from z_bar), where all active variables are random
- Real beta (const RealVector &x, bool cdf_flag, Real z_bar)

  return the reliability index (mapped from z_bar), treating a subset of variables as random
- Real combined_beta (bool cdf_flag, Real z_bar)

  return the reliability index (mapped from z_bar), where all active variables are random
- Real combined_beta (const RealVector &x, bool cdf_flag, Real z_bar)

  return the reliability index (mapped from z_bar), treating a subset of variables as random
- Real delta_mean ()

  return the change in mean resulting from expansion refinement, where all active variables are random
- Real delta_mean (const RealVector &x)

  return the change in mean resulting from expansion refinement, treating a subset of variables as random
- Real delta_combined_mean ()

  return the change in mean resulting from combined expansion refinement, where all active variables are random
- Real delta_combined_mean (const RealVector &x)

  return the change in mean resulting from combined expansion refinement, treating a subset of variables as random
- Real delta_std_deviation ()

  return the change in standard deviation resulting from expansion refinement, where all active variables are random
- Real delta_std_deviation (const RealVector &x)

  return the change in standard deviation resulting from expansion refinement, treating a subset of variables as random
- Real delta_combined_std_deviation ()

  return the change in standard deviation resulting from combined expansion refinement, where all active variables are random
- Real delta_combined_std_deviation (const RealVector &x)

  return the change in standard deviation resulting from combined expansion refinement, treating a subset of variables as random
- Real delta_variance ()

return the change in variance resulting from expansion refinement, where all active variables are random

- Real delta_variance (const RealVector &x)

  return the change in variance resulting from expansion refinement, treating a subset of variables as random

- Real delta_combined_variance ()

  return the change in variance resulting from combined expansion refinement, where all active variables are random

- Real delta_combined_variance (const RealVector &x)

  return the change in variance resulting from combined expansion refinement, treating a subset of variables as random

- Real delta_covariance (Approximation &approx_2)

  return the change in covariance resulting from expansion refinement, where all active variables are random

- Real delta_covariance (const Pecos::RealVector &x, Approximation &approx_2)

  return the change in covariance resulting from expansion refinement, where a subset of the active variables are random

- Real delta_combined_covariance (Approximation &approx_2)

  return the change in covariance resulting from expansion refinement, where all active variables are random

- Real delta_combined_covariance (const Pecos::RealVector &x, Approximation &approx_2)

  return the change in covariance resulting from expansion refinement, where a subset of the active variables are random

- Real delta_beta (bool cdf_flag, Real z_bar)

  return the change in reliability index (mapped from z_bar) resulting from expansion refinement, where all active variables are random

- Real delta_beta (const RealVector &x, bool cdf_flag, Real z_bar)

  return the change in reliability index (mapped from z_bar) resulting from expansion refinement, treating a subset of variables as random

- Real delta_combined_beta (bool cdf_flag, Real z_bar)

  return the change in reliability index (mapped from z_bar) resulting from expansion refinement, where all active variables are random

- Real delta_combined_beta (const RealVector &x, bool cdf_flag, Real z_bar)

  return the change in reliability index (mapped from z_bar) resulting from expansion refinement, treating a subset of variables as random

- Real delta_z (bool cdf_flag, Real beta_bar)

  return the change in response level (mapped from beta_bar) resulting from expansion refinement, where all active variables are random

- Real delta_z (const RealVector &x, bool cdf_flag, Real beta_bar)

  return the change in response level (mapped from beta_bar) resulting from expansion refinement, where a subset of the active variables are random

- Real delta_combined_z (bool cdf_flag, Real beta_bar)

  return the change in response level (mapped from beta_bar) resulting from expansion refinement, where all active variables are random

- Real delta_combined_z (const RealVector &x, bool cdf_flag, Real beta_bar)

  return the change in response level (mapped from beta_bar) resulting from expansion refinement, where a subset of the active variables are random

- void compute_moments (bool full_stats=true, bool combined_stats=false)

  compute moments up to the order supported by the Pecos polynomial approximation

- void compute_moments (const Pecos::RealVector &x, bool full_stats=true, bool combined_stats=false)

  compute moments in all-variables mode up to the order supported by the Pecos polynomial approximation

- const RealVector & moments () const

  return primary moments using Pecos::PolynomialApproximation::moments()

- const RealVector & expansion_moments () const

  return expansion moments from Pecos::PolynomialApproximation

- const RealVector & numerical_integration_moments () const

  return numerical moments from Pecos::PolynomialApproximation

- const RealVector & combined_moments () const

  return combined moments from multilevel-muktifidelity expansion roll-up

- Real moment (size_t i) const

  return primary moment using Pecos::PolynomialApproximation::moment(i)
- void moment (Real mom, size_t i)

  set primary moment using Pecos::PolynomialApproximation::moment(i)
- Real combined_moment (size_t i) const

  return Pecos::PolynomialApproximation::combinedMoments[i]
- void combined_moment (Real mom, size_t i)

  set Pecos::PolynomialApproximation::combinedMoments[i]
- void clear_computed_bits ()

  clear tracking of computed moments, due to a change that invalidates previous results
- void build_linear_system (RealMatrix &A, const UShort2DArray &multi_index)

  construct the Vandermonde matrix "A" for PCE regression for Ax = b
- void **augment_linear_system** (const RealVectorArray &samples, RealMatrix &A, const UShort2DArray &multi_index)
- Pecos::BasisApproximation & pecos_basis_approximation ()

  return pecosBasisApprox

Protected Member Functions

- void active_model_key (const Pecos::ActiveKey &key)

  assign active key in approxData and update_active_iterators()
- Real value (const Variables &vars)

  retrieve the approximate function value for a given parameter vector
- const Pecos::RealVector & gradient (const Variables &vars)

  retrieve the approximate function gradient for a given parameter vector
- const Pecos::RealSymMatrix & hessian (const Variables &vars)

  retrieve the approximate function Hessian for a given parameter vector
- int min_coefficients () const

  return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- void build ()

  builds the approximation from scratch
- void rebuild ()

  rebuilds the approximation incrementally
- void pop_coefficients (bool save_data)

  removes entries from end of SurrogateData::{vars,resp}Data (last points appended, or as specified in args)
- void push_coefficients ()

  restores state prior to previous pop()
- void finalize_coefficients ()

  finalize approximation by applying all remaining trial sets
- void combine_coefficients ()

  combine all level approximations into a single aggregate approximation
- void combined_to_active_coefficients (bool clear_combined=true)

  promote combined approximation into active approximation
- void clear_inactive_coefficients ()

  prune inactive coefficients following combination and promotion to active
- bool advancement_available ()

  check if resolution advancement (e.g., order, rank) is available for this approximation instance
- void print_coefficients (std::ostream &s, bool normalized)

  print the coefficient array computed in build()/rebuild()
- RealVector approximation_coefficients (bool normalized) const

return expansion coefficients in a form consistent with the shared multi-index

- void approximation_coefficients (const RealVector &approx_coeffs, bool normalized)

  set expansion coefficients in a form consistent with the shared multi-index
- void coefficient_labels (std::vector< std::string > &coeff_labels) const

  print the coefficient array computed in build()/rebuild()

Private Member Functions

- void approx_type_to_basis_type (const String &approx_type, short &basis_type)

  utility to convert Dakota type string to Pecos type enumeration

Private Attributes

- Pecos::BasisApproximation pecosBasisApprox

  the Pecos basis approximation, encompassing orthogonal and interpolation polynomial approximations
- std::shared_ptr
  < Pecos::PolynomialApproximation > polyApproxRep

  convenience pointer to representation of Pecos polynomial approximation

Additional Inherited Members

14.204.1 Detailed Description

Derived approximation class for global basis polynomials.

The PecosApproximation class provides a global approximation based on basis polynomials. This includes orthogonal polynomials used for polynomial chaos expansions and interpolation polynomials used for stochastic collocation.

14.204.2 Member Function Documentation

14.204.2.1 void build ( ) [inline], [protected], [virtual]

builds the approximation from scratch

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

References Approximation::build(), and PecosApproximation::pecosBasisApprox.

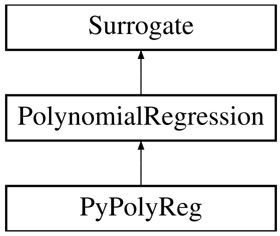
The documentation for this class was generated from the following files:

- PecosApproximation.hpp
- PecosApproximation.cpp

14.205 PolynomialRegression Class Reference

The PolynomialRegression class constructs a polynomial regressor using ordinary least squares.

Inheritance diagram for PolynomialRegression:



Public Member Functions

- PolynomialRegression ()

  Constructor that uses defaultConfigOptions and does not build.
- PolynomialRegression (const ParameterList &options)

  Constructor that sets configOptions and does not build.
- PolynomialRegression (const std::string &param_list_yaml_filename)

  Constructor for the PolynomialRegression class that sets configOptions but does not build the surrogate.
- PolynomialRegression (const MatrixXd &samples, const MatrixXd &response, const ParameterList &options)

  Constructor sets configOptions and builds the Polynomial Regression surrogate.
- PolynomialRegression (const MatrixXd &samples, const MatrixXd &response, const std::string &param_list-_yaml_filename)

  Constructor for the PolynomialRegression class that sets configOptions and builds the surrogate.
- ∼PolynomialRegression ()

  Default destructor.
- void compute_basis_matrix (const MatrixXd &samples, MatrixXd &basis_matrix) const

  Constructs a basis matrix for a set of samples according to the member variable basisIndices.
- void build (const MatrixXd &samples, const MatrixXd &response) override

  Build the polynomial surrogate using specified build data.
- VectorXd value (const MatrixXd &eval_points, const int qoi) override

  Evaluate the polynomial surrogate at a set of prediction points for a single QoI.
- VectorXd value (const MatrixXd &eval_points)

  Evaluate the polynomial surrogate at a set of prediction points for QoI index 0.
- MatrixXd gradient (const MatrixXd &eval_points, const int qoi) override

  Evaluate the gradient of the polynomial surrogate at a set of prediction points for a single QoI.
- MatrixXd gradient (const MatrixXd &eval_points)

  Evaluate the gradient of the polynomial surrogate at a set of prediction points for QoI index 0.
- MatrixXd hessian (const MatrixXd &eval_point, const int qoi) override

  Evaluate the Hessian of the polynomial surrogate at a single point for a single QoI.
- MatrixXd hessian (const MatrixXd &eval_point)

  Evaluate the Hessian of the polynomial surrogate at a single point for QoI index 0.
- const MatrixXd & get_polynomial_coeffs () const

  Get the polynomial surrogate's coefficients.
- double get_polynomial_intercept () const

  Get the polynomial surrogate's intercept/offset.
- int get_num_terms () const

  Get the number of terms in the polynomial surrogate.
- void set_polynomial_coeffs (const MatrixXd &coeffs)

  Set the polynomial surrogate's coefficients.
- std::shared_ptr< Surrogate > clone () const override

  clone derived Surrogate class for use in cross-validation

Private Member Functions

- void default_options () override

  Construct and populate the defaultConfigOptions.

- template<class Archive >
  void serialize (Archive &archive, const unsigned int version)

  Serializer for save/load.

Private Attributes

- MatrixXi basisIndices

  Matrix that specifies the powers of each variable for each term in the polynomial - (numVariables by numTerms).

- std::shared_ptr
  < util::LinearSolverBase > linearSolver

  Linear solver for the ordinary least squares problem.

- int numTerms

  Number of terms in the polynomial basis.

- MatrixXd polynomialCoeffs

  Vector of coefficients for the polynomial surrogate.

- double polynomialIntercept

  Offset/intercept term for the polynomial surrogate.

- int verbosity

  Verbosity level.

Friends

- class boost::serialization::access

  Allow serializers access to private class data.

Additional Inherited Members

14.205.1 Detailed Description

The PolynomialRegression class constructs a polynomial regressor using ordinary least squares.

Users may specify the max degree and p-norm for a hyperbolic cross scheme to specify the terms in the polynomial basis. A p-norm = 1 results in a total order specification of max degree.

The DataScaler class provides the option of scaling the basis matrix.

14.205.2 Constructor & Destructor Documentation

14.205.2.1 PolynomialRegression (const ParameterList & *options*)

Constructor that sets configOptions and does not build.

Parameters

in	*options*	List that overrides entries in defaultConfigOptions.

References Surrogate::configOptions, PolynomialRegression::default_options(), and Surrogate::defaultConfigOptions.

14.205.2.2 PolynomialRegression (const std::string & *param_list_yaml_filename*)

Constructor for the PolynomialRegression class that sets configOptions but does not build the surrogate.

Parameters

in	*param_list_yaml-_filename*	A ParameterList file (relative to the location of the Dakota input file) that overrides entries in defaultConfigOptions.

References Surrogate::configOptions, PolynomialRegression::default_options(), and Surrogate::defaultConfigOptions.

14.205.2.3 PolynomialRegression (const MatrixXd & *samples,* const MatrixXd & *response,* const ParameterList & *options*)

Constructor sets configOptions and builds the Polynomial Regression surrogate.

Parameters

in	*samples*	Matrix of data for surrogate construction - (num_samples by num_features)
in	*response*	Vector of targets for surrogate construction - (num_samples by num_qoi = 1; only 1 response is supported currently).
in	*options*	List that overrides entries in defaultConfigOptions

References PolynomialRegression::build(), Surrogate::configOptions, and PolynomialRegression::default_options().

14.205.2.4 PolynomialRegression (const MatrixXd & *samples,* const MatrixXd & *response,* const std::string & *param_list_yaml_filename*)

Constructor for the PolynomialRegression class that sets configOptions and builds the surrogate.

Parameters

in	*samples*	Matrix of data for surrogate construction - (num_samples by num_features)
in	*response*	Vector of targets for surrogate construction - (num_samples by num_qoi = 1; only 1 response is supported currently).
in	*param_list_yaml-_filename*	A ParameterList file (relative to the location of the Dakota input file) that overrides entries in defaultConfigOptions.

References PolynomialRegression::build(), Surrogate::configOptions, and PolynomialRegression::default_options().

14.205.3 Member Function Documentation

14.205.3.1 void compute_basis_matrix (const MatrixXd & *samples,* MatrixXd & *basis_matrix*) const

Constructs a basis matrix for a set of samples according to the member variable basisIndices.

Parameters

in	*samples*	Matrix of sample points - (num_points by num_features).
out	*basis_matrix*	Matrix that contains polynomial basis function evaluations in its rows for each sample point - (num_points by numTerms), numTerms being the number of terms in the polynomial basis.

References PolynomialRegression::basisIndices, PolynomialRegression::numTerms, and Surrogate::numVariables.

Referenced by PolynomialRegression::build(), PolynomialRegression::gradient(), PolynomialRegression::hessian(), and PolynomialRegression::value().

14.205.3.2 void build (const MatrixXd & *samples,* const MatrixXd & *response*) [override], [virtual]

Build the polynomial surrogate using specified build data.

Parameters

in	*samples*	Matrix of data for surrogate construction - (num_samples by num_features)
in	*response*	Vector of targets for surrogate construction - (num_samples by num_qoi = 1; only 1 response is supported currently).

Implements Surrogate.

References PolynomialRegression::basisIndices, PolynomialRegression::compute_basis_matrix(), dakota::surrogates::compute_hyperbolic_indices(), dakota::surrogates::compute_reduced_indices(), Surrogate::configOptions, Surrogate::dataScaler, Surrogate::defaultConfigOptions, PolynomialRegression::linearSolver, Surrogate::numQOI, Surrogate::numSamples, PolynomialRegression::numTerms, Surrogate::numVariables, PolynomialRegression::polynomialCoeffs, PolynomialRegression::polynomialIntercept, Surrogate::responseOffset, Surrogate::responseScaleFactor, DataScaler::scale_samples(), dakota::util::scaler_factory(), DataScaler::scaler_type(), dakota::util::solver_factory(), LinearSolverBase::solver_type(), and PolynomialRegression::verbosity.

Referenced by PolynomialRegression::PolynomialRegression().

14.205.3.3 VectorXd value (const MatrixXd & *eval_points,* const int *qoi*) [override], [virtual]

Evaluate the polynomial surrogate at a set of prediction points for a single QoI.

Parameters

in	*eval_points*	Matrix of prediction points - (num_pts by num_features).
in	*qoi*	Index for surrogate QoI.

Returns

Values of the polynomial surrogate at the prediction points - (num_pts)

Implements Surrogate.

References PolynomialRegression::compute_basis_matrix(), Surrogate::dataScaler, PolynomialRegression::polynomialCoeffs, PolynomialRegression::polynomialIntercept, Surrogate::responseOffset, Surrogate::responseScaleFactor, DataScaler::scale_samples(), and dakota::silence_unused_args().

14.205.3.4 VectorXd value (const MatrixXd & *eval_points*) [inline]

Evaluate the polynomial surrogate at a set of prediction points for QoI index 0.

Parameters

in	*eval_points*	Matrix of prediction points - (num_pts by num_features).

Returns

Values of the polynomial surrogate at the prediction points - (num_pts)

References Surrogate::value().

14.205.3.5 MatrixXd gradient (const MatrixXd & *eval_points,* const int *qoi*) [override], [virtual]

Evaluate the gradient of the polynomial surrogate at a set of prediction points for a single QoI.

Parameters

in	*eval_points*	Coordinates of the prediction points - (num_pts by num_features).
in	*qoi*	Index of response/QOI for which to compute derivatives.

Returns

Matrix of gradient vectors at the prediction points - (num_pts by num_features).

Reimplemented from Surrogate.

References PolynomialRegression::basisIndices, PolynomialRegression::compute_basis_matrix(), Surrogate::dataScaler, PolynomialRegression::numTerms, Surrogate::numVariables, PolynomialRegression::polynomialCoeffs, Surrogate::responseScaleFactor, DataScaler::scale_samples(), and dakota::silence_unused_args().

14.205.3.6 MatrixXd gradient (const MatrixXd & *eval_points*) [inline]

Evaluate the gradient of the polynomial surrogate at a set of prediction points for QoI index 0.

Parameters

in	*eval_points*	Coordinates of the prediction points - (num_pts by num_features).

Returns

Matrix of gradient vectors at the prediction points - (num_pts by num_features).

References Surrogate::gradient().

14.205.3.7 MatrixXd hessian (const MatrixXd & *eval_point,* const int *qoi*) [override], [virtual]

Evaluate the Hessian of the polynomial surrogate at a single point for a single QoI.

Parameters

in	*eval_point*	Coordinates of the prediction point - (1 by num_features).
in	*qoi*	Index of response/QOI for which to compute derivatives.

Returns

Hessian matrix at the prediction point - (num_features by num_features).

Reimplemented from Surrogate.

References PolynomialRegression::basisIndices, PolynomialRegression::compute_basis_matrix(), Surrogate::dataScaler, PolynomialRegression::numTerms, Surrogate::numVariables, PolynomialRegression::polynomialCoeffs, Surrogate::responseScaleFactor, DataScaler::scale_samples(), and dakota::silence_unused_args().

14.205.3.8 MatrixXd hessian (const MatrixXd & *eval_point*) [inline]

Evaluate the Hessian of the polynomial surrogate at a single point for QoI index 0.

Parameters

in	*eval_point*	Coordinates of the prediction point - (1 by num_features).

Returns

Hessian matrix at the prediction point - (num_features by num_features).

References Surrogate::hessian().

The documentation for this class was generated from the following files:

- SurrogatesPolynomialRegression.hpp
- SurrogatesPolynomialRegression.cpp

14.206 PrefixingLineFilter Class Reference

Inherits line_filter.

Public Member Functions

- PrefixingLineFilter (const std::string &prefix_in)

  Constructor.

Private Member Functions

- std::string do_filter (const std::string &line)

  "Filter" the line by adding the prefix

Private Attributes

- std::string linePrefix

  Prefix for each line.

14.206.1 Detailed Description

PrefixingLineFilter is dervied from a Boost stream filter class in order to preface output with specified text. In this case, the intent is to distinguish ROL output.

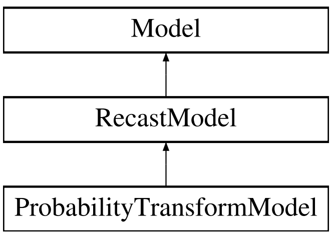
The documentation for this class was generated from the following file:

- ROLOptimizer.hpp

14.207 ProbabilityTransformModel Class Reference

Probability transformation specialization of RecastModel.

Inheritance diagram for ProbabilityTransformModel:



Public Member Functions

- ProbabilityTransformModel (const Model &sub_model, short u_space_type, bool truncate_bnds=false, Real bnd=10.)

  standard constructor
- ∼ProbabilityTransformModel ()

  destructor

Static Public Member Functions

- static void initialize_distribution_types (short u_space_type, const Pecos::MultivariateDistribution &x_dist, Pecos::MultivariateDistribution &u_dist)

  initialize transformed distribution types and instantiate mvDist

Protected Member Functions

- Pecos::ProbabilityTransformation & probability_transformation ()

  return probability transformation employed by the Model (forwarded along to ProbabilityTransformModel recasting)
- bool resize_pending () const

  return true if a potential resize is still pending, such that sizing-based initialization should be deferred
- void update_from_subordinate_model (size_t depth=SZ_MAX)

  propagate vars/labels/bounds/targets from the bottom up
- void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

  set primaryACVarMapIndices and secondaryACVarMapTargets (only, for now)
- const SizetArray & nested_acv1_indices () const

  return primaryACVarMapIndices
- const ShortArray & nested_acv2_targets () const

  return secondaryACVarMapTargets
- short query_distribution_parameter_derivatives () const

  calculate and return potential state of distribution parameter derivatives, but do not cache value in distParamDerivs
- void activate_distribution_parameter_derivatives ()

  activate distParamDerivs to {NO,MIXED,ALL}_DERIVS
- void deactivate_distribution_parameter_derivatives ()

  reset distParamDerivs to NO_DERIVS
- void assign_instance ()

  assign static pointer instance to this for use in static transformation functions
- void init_metadata () override

  default clear metadata in Recasts; derived classes can override to no-op
- void trans_grad_X_to_U (const RealVector &fn_grad_x, RealVector &fn_grad_u, const RealVector &x_vars)

  transform x-space gradient vector to u-space
- void trans_grad_U_to_X (const RealVector &fn_grad_u, RealVector &fn_grad_x, const RealVector &x_vars)

  transform u-space gradient vector to x-space
- void trans_grad_X_to_S (const RealVector &fn_grad_x, RealVector &fn_grad_s, const RealVector &x_vars)

  transform x-space gradient vector to gradient with respect to inserted distribution parameters
- void trans_hess_X_to_U (const RealSymMatrix &fn_hess_x, RealSymMatrix &fn_hess_u, const RealVector &x_vars, const RealVector &fn_grad_x)

  transform x-space Hessian matrix to u-space
- void initialize_transformation (short u_space_type)

  initialize transformed distribution types and natafTransform (construct time)

- void update_transformation ()

  update with latest distribution data (run time)
- void initialize_nataf ()

  instantiate and initialize natafTransform
- void verify_correlation_support (short u_space_type)

  verify that correlation warping is supported by Nataf for given variable types
- void initialize_dakota_variable_types ()

  initialize the continuous/discrete variable types using u-space types (converted from Pecos to Dakota)
- void update_model_bounds (bool truncate_bnds, Real bnd)

  update model bounds using u-space (truncated) distribution bounds
- bool nonlinear_variables_mapping (const Pecos::MultivariateDistribution &x_dist, const Pecos::Multivariate-Distribution &u_dist) const

  detect when the variables transformation is nonlinear
- size_t rv_index_to_corr_index (size_t rv_index)

  convert vector<RandomVariable> index to active correlation index
- size_t acv_index_to_corr_index (size_t acv_index)

  convert allContinuousVars index to active correlation index
- unsigned short pecos_to_dakota_variable_type (unsigned short pecos_var_type, size_t rv_index)

  convert from Pecos To Dakota variable enumeration type for continuous aleatory uncertain variables used in variable transformations

Static Protected Member Functions

- static void vars_u_to_x_mapping (const Variables &u_vars, Variables &x_vars)

  static function for RecastModels used for forward mapping of u-space variables from NonD Iterators to x-space variables for Model evaluations
- static void vars_x_to_u_mapping (const Variables &x_vars, Variables &u_vars)

  static function for RecastModels used for inverse mapping of x-space variables from data import to u-space variables for NonD Iterators
- static void set_u_to_x_mapping (const Variables &u_vars, const ActiveSet &u_set, ActiveSet &x_set)

  static function for RecastModels used to map u-space ActiveSets from NonD Iterators to x-space ActiveSets for Model evaluations
- static void resp_x_to_u_mapping (const Variables &x_vars, const Variables &u_vars, const Response &x_-response, Response &u_response)

  static function for RecastModels used to map x-space responses from Model evaluations to u-space responses for return to NonD Iterator.

Private Attributes

- Pecos::ProbabilityTransformation natafTransform

  Nonlinear variable transformation that encapsulates the required data for performing transformations from X -> Z -> U and back.
- short distParamDerivs

  indicates state of derivatives of final results with respect to distribution parameters s within resp_x_to_u_mapping() using the chain rule df/dx dx/ds. The default is to calculate derivatives with respect to standard random variables u using the chain rule df/dx dx/du.
- bool truncatedBounds

  boolean flag indicating use of distribution truncation for defining global model bounds
- Real boundVal

  number of +/- standard deviations used for defining bounds truncation
- SizetArray primaryACVarMapIndices

  "primary" all continuous variable mapping indices flowed down from higher level iteration
- ShortArray secondaryACVarMapTargets

  "secondary" all continuous variable mapping targets flowed down from higher level iteration

Static Private Attributes

- static ProbabilityTransformModel * ptmInstance

  static pointer to this class for use in static callbacks

Additional Inherited Members

14.207.1 Detailed Description

Probability transformation specialization of RecastModel.

Specialization of RecastModel to transform a sub-model to u-space.

14.207.2 Member Function Documentation

14.207.2.1 void initialize_distribution_types (short *u_space_type,* const Pecos::MultivariateDistribution & *x_dist,* Pecos::MultivariateDistribution & *u_dist*) [static]

initialize transformed distribution types and instantiate mvDist

Build ProbabilityTransformation::ranVar arrays containing the uncertain variable distribution types and their corresponding means/standard deviations. This function is used when the Model variables are in x-space.

References Dakota::abort_handler().

Referenced by NonDLHSSampling::d_optimal_parameter_set(), and ProbabilityTransformModel::initialize_-transformation().

14.207.2.2 void update_from_subordinate_model (size_t *depth* = SZ_MAX) [inline], [protected], [virtual]

propagate vars/labels/bounds/targets from the bottom up

used only for instantiate-on-the-fly model recursions (all RecastModel instantiations and alternate DataFitSurrModel instantiations). Simulation, Hierarchical, and Nested Models do not redefine the function since they do not support instantiate-on-the-fly. This means that the recursion will stop as soon as it encounters a Model that was instantiated normally, which is appropriate since ProblemDescDB-constructed Models use top-down information flow and do not require bottom-up updating.

Reimplemented from Model.

References RecastModel::subModel, Dakota::SZ_MAX, RecastModel::update_from_model(), Model::update_from-_subordinate_model(), and ProbabilityTransformModel::update_transformation().

14.207.2.3 void vars_u_to_x_mapping (const Variables & *u_vars,* Variables & *x_vars*) [inline], [static], [protected]

static function for RecastModels used for forward mapping of u-space variables from NonD Iterators to x-space variables for Model evaluations

Map the variables from iterator space (u) to simulation space (x).

References Variables::continuous_variables(), Variables::continuous_variables_view(), ProbabilityTransformModel-::natafTransform, and ProbabilityTransformModel::ptmInstance.

Referenced by ProbabilityTransformModel::ProbabilityTransformModel().

14.207.2.4 void vars_x_to_u_mapping (const Variables & *x_vars*, Variables & *u_vars*) [inline], [static], [protected]

static function for RecastModels used for inverse mapping of x-space variables from data import to u-space variables for NonD Iterators

Map the variables from simulation space (x) to iterator space (u).

References Variables::continuous_variables(), Variables::continuous_variables_view(), ProbabilityTransformModel::natafTransform, and ProbabilityTransformModel::ptmInstance.

Referenced by ProbabilityTransformModel::ProbabilityTransformModel().

14.207.2.5 void set_u_to_x_mapping (const Variables & *u_vars*, const ActiveSet & *u_set*, ActiveSet & *x_set*) [static], [protected]

static function for RecastModels used to map u-space ActiveSets from NonD Iterators to x-space ActiveSets for Model evaluations

Define the DVV for x-space derivative evaluations by augmenting the iterator requests to account for correlations.

References ProbabilityTransformModel::acv_index_to_corr_index(), Variables::all_continuous_variable_ids(), Dakota::contains(), Variables::continuous_variable_ids(), ActiveSet::derivative_vector(), Variables::inactive_continuous_variable_ids(), Model::multivariate_distribution(), ProbabilityTransformModel::ptmInstance, and RecastModel::subModel.

Referenced by ProbabilityTransformModel::ProbabilityTransformModel().

14.207.3 Member Data Documentation

14.207.3.1 ProbabilityTransformModel ∗ ptmInstance [static], [private]

static pointer to this class for use in static callbacks

initialization of static needed by RecastModel

Referenced by ProbabilityTransformModel::assign_instance(), ProbabilityTransformModel::resp_x_to_u_mapping(), ProbabilityTransformModel::set_u_to_x_mapping(), ProbabilityTransformModel::vars_u_to_x_mapping(), and ProbabilityTransformModel::vars_x_to_u_mapping().

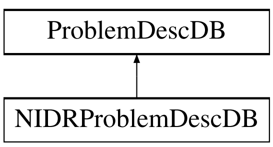
The documentation for this class was generated from the following files:

- ProbabilityTransformModel.hpp
- ProbabilityTransformModel.cpp

14.208 ProblemDescDB Class Reference

The database containing information parsed from the DAKOTA input file.

Inheritance diagram for ProblemDescDB:



Public Member Functions

- ProblemDescDB ()

  default constructor
- ProblemDescDB (ParallelLibrary &parallel_lib)

  standard constructor
- ProblemDescDB (const ProblemDescDB &db)

  copy constructor
- ∼ProblemDescDB ()

  destructor
- ProblemDescDB operator= (const ProblemDescDB &db)

  assignment operator
- void parse_inputs (ProgramOptions &prog_opts, DbCallbackFunctionPtr callback=NULL, void ∗callback_-data=NULL)

  Parses the input file or input string if present and executes callbacks. Does not perform any validation.
- void check_and_broadcast (const ProgramOptions &prog_opts)

  performs check_input, broadcast, and post_process, but for now, allowing separate invocation through the public API as well
- void check_input ()

  verifies that there is at least one of each of the required keywords in the dakota input file
- void broadcast ()

  invokes send_db_buffer() and receive_db_buffer() to broadcast DB data across the processor allocation. Used by manage_inputs().
- void post_process ()

  post-processes the (minimal) input specification to assign default variables/responses specification arrays. Used by manage_inputs().
- void lock ()

  Locks the database in order to prevent data access when the list nodes may not be set properly. Unlocked by a set nodes operation.
- void unlock ()

  Explicitly unlocks the database. Use with care.
- void set_db_list_nodes (const String &method_tag)

  set dataMethodIter based on a method identifier string to activate a particular method specification in dataMethodList and use pointers from this method specification to set all other list iterators.
- void set_db_list_nodes (size_t method_index)

  set dataMethodIter based on an index within dataMethodList to activate a particular method specification and use pointers from this method specification to set all other list iterators.
- void resolve_top_method (bool set_model_nodes=true)

  For a (default) environment lacking a top method pointer, this function is used to determine which of several potential method specifications corresponds to the top method and then sets the list nodes accordingly.
- void set_db_method_node (const String &method_tag)

  set dataMethodIter based on a method identifier string to activate a particular method specification (only).
- void set_db_method_node (size_t method_index)

  set dataMethodIter based on an index within dataMethodList to activate a particular method specification (only).
- size_t get_db_method_node ()

  return the index of the active node in dataMethodList
- void set_db_model_nodes (const String &model_tag)

  set the model list iterators (dataModelIter, dataVariablesIter, dataInterfaceIter, and dataResponsesIter) based on the model identifier string
- void set_db_model_nodes (size_t model_index)

  set the model list iterators (dataModelIter, dataVariablesIter, dataInterfaceIter, and dataResponsesIter) based on an index within dataModelList
- size_t get_db_model_node ()

return the index of the active node in dataModelList
- void set_db_variables_node (const String &variables_tag)

  set dataVariablesIter based on the variables identifier string
- void set_db_interface_node (const String &interface_tag)

  set dataInterfaceIter based on the interface identifier string
- void set_db_responses_node (const String &responses_tag)

  set dataResponsesIter based on the responses identifier string
- ParallelLibrary & parallel_library () const

  return the parallelLib reference
- IteratorList & iterator_list ()

  return a list of all Iterator objects that have been instantiated
- ModelList & model_list ()

  return a list of all Model objects that have been instantiated
- VariablesList & variables_list ()

  return a list of all Variables objects that have been instantiated
- InterfaceList & interface_list ()

  return a list of all Interface objects that have been instantiated
- ResponseList & response_list ()

  return a list of all Response objects that have been instantiated
- const RealMatrixArray & get_rma (const String &entry_name) const

  get a RealMatrixArray out of the database based on an identifier string
- const RealVector & get_rv (const String &entry_name) const

  get a RealVector out of the database based on an identifier string
- const IntVector & get_iv (const String &entry_name) const

  get an IntVector out of the database based on an identifier string
- const BitArray & get_ba (const String &entry_name) const

  get a BitArray out of the database based on an identifier string
- const SizetArray & get_sza (const String &entry_name) const

  get an SizetArray out of the database based on an identifier string
- const UShortArray & get_usa (const String &entry_name) const

  get an UShortArray out of the database based on an identifier string
- const RealSymMatrix & get_rsm (const String &entry_name) const

  get a RealSymMatrix out of the database based on an identifier string
- const RealVectorArray & get_rva (const String &entry_name) const

  get a RealVectorArray out of the database based on an identifier string
- const IntVectorArray & get_iva (const String &entry_name) const

  get an IntVectorArray out of the database based on an identifier string
- const IntSet & get_is (const String &entry_name) const

  get an IntSet out of the database based on an identifier string
- const IntSetArray & get_isa (const String &entry_name) const

  get an IntSetArray out of the database based on an identifier string
- const SizetSet & get_szs (const String &entry_name) const

  get a SizetSet out of the database based on an identifier string
- const StringSetArray & get_ssa (const String &entry_name) const

  get an StringSetArray out of the database based on an identifier string
- const RealSetArray & get_rsa (const String &entry_name) const

  get a RealSetArray out of the database based on an identifier string
- const IntRealMapArray & get_irma (const String &entry_name) const

  get an IntRealMapArray out of the database based on an identifier string
- const StringRealMapArray & get_srma (const String &entry_name) const

  get an StringRealMapArray out of the database based on an identifier string

- const RealRealMapArray & get_rrma (const String &entry_name) const

  get a RealRealMapArray out of the database based on an identifier string
- const RealRealPairRealMapArray & get_rrrma (const String &entry_name) const

  get a RealRealPairRealMapArray out of the database based on an identifier string
- const IntIntPairRealMapArray & get_iirma (const String &entry_name) const

  get an IntIntPairRealMapArray out of the database based on an identifier string
- const StringArray & get_sa (const String &entry_name) const

  get a StringArray out of the database based on an identifier string
- const String2DArray & get_s2a (const String &entry_name) const

  get a String2DArray out of the database based on an identifier string
- const String & get_string (const String &entry_name) const

  get a String out of the database based on an identifier string
- const Real & get_real (const String &entry_name) const

  get a Real out of the database based on an identifier string
- int get_int (const String &entry_name) const

  get an int out of the database based on an identifier string
- short get_short (const String &entry_name) const

  get a short out of the database based on an identifier string
- unsigned short get_ushort (const String &entry_name) const

  get an unsigned short out of the database based on an identifier string
- size_t get_sizet (const String &entry_name) const

  get a size_t out of the database based on an identifier string
- bool get_bool (const String &entry_name) const

  get a bool out of the database based on an identifier string
- void ** get_voidss (const String &entry_name) const

  *for getting a void**, e.g., &dlLib*
- void insert_node (const DataEnvironment &data_env)

  set the DataEnvironment object
- void insert_node (const DataMethod &data_method)

  add a DataMethod object to the dataMethodList
- void insert_node (const DataModel &data_model)

  add a DataModel object to the dataModelList
- void insert_node (DataVariables &data_variables)

  add a DataVariables object to the dataVariablesList
- void insert_node (const DataInterface &data_interface)

  add a DataInterface object to the dataInterfaceList
- void insert_node (const DataResponses &data_responses)

  add a DataResponses object to the dataResponsesList
- void set (const String &entry_name, const RealVector &rv)

  set a RealVector within the database based on an identifier string
- void set (const String &entry_name, const IntVector &iv)

  set an IntVector within the database based on an identifier string
- void set (const String &entry_name, const BitArray &ba)

  set a BitArray within the database based on an identifier string
- void set (const String &entry_name, const RealSymMatrix &rsm)

  set a RealMatrix within the database based on an identifier string
- void set (const String &entry_name, const RealVectorArray &rva)

  set a RealVectorArray within the database based on an identifier string
- void set (const String &entry_name, const IntVectorArray &iva)

  set an IntVectorArray within the database based on an identifier string
- void set (const String &entry_name, const IntSetArray &isa)

set an IntSetArray within the database based on an identifier string

- void set (const String &entry_name, const RealSetArray &rsa)

  set a RealSetArray within the database based on an identifier string

- void set (const String &entry_name, const IntRealMapArray &irma)

  set an IntRealMapArray within the database based on an identifier string

- void set (const String &entry_name, const StringRealMapArray &srma)

  set a StringRealMapArray within the database based on an identifier string

- void set (const String &entry_name, const RealRealMapArray &rrma)

  set a RealRealMapArray within the database based on an identifier string

- void set (const String &entry_name, const RealRealPairRealMapArray &iirma)

  set a RealRealPairRealMapArray in the db based on an identifier string

- void set (const String &entry_name, const IntIntPairRealMapArray &iirma)

  set an IntIntPairRealMapArray in the db based on an identifier string

- void set (const String &entry_name, const StringArray &sa)

  set a StringArray within the database based on an identifier string

- int min_procs_per_ea ()

  compute minimum evaluation partition size based on lower level overrides

- int max_procs_per_ea ()

  compute maximum evaluation partition size based on lower level overrides and concurrency levels

- int min_procs_per_ie ()

  compute minimum iterator partition size based on lower level overrides

- int max_procs_per_ie (int max_eval_concurrency)

  compute maximum iterator partition size based on lower level overrides and concurrency levels

- bool method_locked () const

  return methodDBLocked

- bool model_locked () const

  return modelDBLocked

- bool variables_locked () const

  return variablesDBLocked

- bool interface_locked () const

  return interfaceDBLocked

- bool responses_locked () const

  return responsesDBLocked

- bool is_null () const

  function to check dbRep (does this envelope contain a letter)

Static Public Member Functions

- static int min_procs_per_level (int min_procs_per_server, int pps_spec, int num_serv_spec)

  compute minimum partition size for a parallel level based on lower level overrides

- static int max_procs_per_level (int max_procs_per_server, int pps_spec, int num_serv_spec, short sched_-spec, int asynch_local_conc, bool peer_dynamic_avail, int max_concurrency)

  compute maximum partition size for a parallel level based on lower level overrides

Protected Member Functions

- ProblemDescDB (BaseConstructor, ParallelLibrary &parallel_lib)

    constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- virtual void derived_parse_inputs (const std::string &dakota_input_file, const std::string &dakota_input_string, const std::string &parser_options)

    derived class specifics within parse_inputs()
- virtual void derived_broadcast ()

    derived class specifics within broadcast()
- virtual void derived_post_process ()

    derived class specifics within post_process()

Protected Attributes

- DataEnvironment environmentSpec

    the environment specification (only one allowed) resulting from a call to environment_kwhandler() or insert_node()
- std::list< DataMethod > dataMethodList

    list of method specifications, one for each call to method_kwhandler() or insert_node()
- std::list< DataModel > dataModelList

    list of model specifications, one for each call to model_kwhandler() or insert_node()
- std::list< DataVariables > dataVariablesList

    list of variables specifications, one for each call to variables_kwhandler() or insert_node()
- std::list< DataInterface > dataInterfaceList

    list of interface specifications, one for each call to interface_kwhandler() or insert_node()
- std::list< DataResponses > dataResponsesList

    list of responses specifications, one for each call to responses_kwhandler() or insert_node()
- size_t environmentCntr

    counter for environment specifications used in check_input

Private Member Functions

- template<typename T >
  T & get (const std::string &context_msg, const std::map< std::string, T DataEnvironmentRep::∗ > &env_map, const std::map< std::string, T DataMethodRep::∗ > &met_map, const std::map< std::string, T DataModelRep::∗ > &mod_map, const std::map< std::string, T DataVariablesRep::∗ > &var_map, const std::map< std::string, T DataInterfaceRep::∗ > &int_map, const std::map< std::string, T DataResponsesRep::∗ > &res_map, const std::string &entry_name, const std::shared_ptr< ProblemDescDB > &db_rep) const

    Encapsulate lookups across Data∗Rep types: given lookup tables mapping strings to pointers to Data∗Rep members, and an entry_name = block.entry_key, return the corresponding member value from the appropriate Data∗Rep in the ProblemDescDB rep.
- const Iterator & get_iterator ()

    retrieve an existing Iterator, if it exists in iteratorList, or instantiate a new one
- const Iterator & get_iterator (Model &model)

    retrieve an existing Iterator, if it exists in iteratorList, or instantiate a new one
- const Iterator & get_iterator (const String &method_name, Model &model)

    retrieve an existing Iterator, if it exists in iteratorByNameList, or instantiate a new one
- const Model & get_model ()

    retrieve an existing Model, if it exists, or instantiate a new one
- const Variables & get_variables ()

    retrieve an existing Variables, if it exists, or instantiate a new one
- const Interface & get_interface ()

retrieve an existing Interface, if it exists, or instantiate a new one

- const Response & get_response (short type, const Variables &vars)

    retrieve an existing Response, if it exists, or instantiate a new one

- std::shared_ptr< ProblemDescDB > get_db (ParallelLibrary &parallel_lib)

    Used by the envelope constructor to instantiate the correct letter class.

- void send_db_buffer ()

    MPI send of a large buffer containing environmentSpec and all objects in dataMethodList, dataModelList, dataVariablesList, dataInterfaceList, and dataResponsesList. Used by manage_inputs().

- void receive_db_buffer ()

    MPI receive of a large buffer containing environmentSpec and all objects in dataMethodList, dataModelList, dataVariablesList, dataInterfaceList, and dataResponsesList. Used by manage_inputs().

- bool model_has_interface (const DataModelRep &model_rep) const

    helper function for determining whether an interface specification should be active, based on model type

- void echo_input_file (const std::string &dakota_input_file, const std::string &dakota_input_string, const std::string &tmpl_qualifier="")

    echo the (potentially) specified input file or string to stdout

- void enforce_unique_ids ()

    require user-specified block identifiers to be unique

Private Attributes

- ParallelLibrary & parallelLib

    reference to the parallel_lib object passed from main

- std::list< DataMethod >::iterator dataMethodIter

    iterator identifying the active list node in dataMethodList

- std::list< DataModel >::iterator dataModelIter

    iterator identifying the active list node in dataModelList

- std::list< DataVariables >
  ::iterator dataVariablesIter

    iterator identifying the active list node in dataVariablesList

- std::list< DataInterface >
  ::iterator dataInterfaceIter

    iterator identifying the active list node in dataInterfaceList

- std::list< DataResponses >
  ::iterator dataResponsesIter

    iterator identifying the active list node in dataResponsesList

- IteratorList iteratorList

    list of iterator objects, one for each method specification

- IteratorList iteratorByNameList

    list of iterator objects, one for each lightweight instantiation by name

- ModelList modelList

    list of model objects, one for each model specification

- VariablesList variablesList

    list of variables objects, one for each variables specification

- InterfaceList interfaceList

    list of interface objects, one for each interface specification

- ResponseList responseList

    list of response objects, one for each responses specification

- bool methodDBLocked

    prevents use of get_<type> retrieval and set_<type> update functions prior to setting the list node for the active method specification

- bool modelDBLocked

prevents use of get_<type> retrieval and set_<type> update functions prior to setting the list node for the active model specification

- bool variablesDBLocked

  prevents use of get_<type> retrieval and set_<type> update functions prior to setting the list node for the active variables specification

- bool interfaceDBLocked

  prevents use of get_<type> retrieval and set_<type> update functions prior to setting the list node for the active interface specification

- bool responsesDBLocked

  prevents use of get_<type> retrieval and set_<type> update functions prior to setting the list node for the active responses specification

- std::shared_ptr< ProblemDescDB > dbRep

  pointer to the letter (initialized only for the envelope)

Friends

- class Model

  Model requires access to get_variables() and get_response()

- class SimulationModel

  SimulationModel requires access to get_interface()

- class HierarchSurrModel

  HierarchSurrModel and NonHierarchSurrModel require access to get_model()

- class **NonHierarchSurrModel**
- class DataFitSurrModel

  DataFitSurrModel requires access to get_iterator() and get_model()

- class NestedModel

  NestedModel requires access to get_interface(), get_response(), get_iterator(), and get_model()

- class **ActiveSubspaceModel**
- class **AdaptedBasisModel**
- class **RandomFieldModel**
- class Environment

  Environment requires access to get_iterator()

- class IteratorScheduler

  Environment requires access to get_iterator()

- class Iterator

  Iterator requires access to get_model()

- class MetaIterator

  Iterator requires access to get_model()

- class SeqHybridMetaIterator

  SeqHybridMetaIterator requires access to get_model()

- class CollabHybridMetaIterator

  CollabHybridMetaIterator requires access to get_model()

- class ConcurrentMetaIterator

  ConcurrentMetaIterator requires access to get_model()

- class SurrBasedLocalMinimizer

  HierarchSurrBasedLocalMinimizer requires access to get_iterator()

- class SurrBasedGlobalMinimizer

  SurrBasedGlobalMinimizer requires access to get_iterator()

- class PebbldMinimizer

  PEBBLMinimizer requires access to get_iterator()

14.208.1 Detailed Description

The database containing information parsed from the DAKOTA input file.

The ProblemDescDB class is a database for DAKOTA input file data that is populated by a parser defined in a derived class. When the parser reads a complete keyword, it populates a data class object (DataEnvironment, DataMethod, DataVariables, DataInterface, or DataResponses) and, for all cases except environment, appends the object to a linked list (dataMethodList, dataVariablesList, dataInterfaceList, or dataResponsesList). No environment linked list is used since only one environment specification is allowed.

14.208.2 Constructor & Destructor Documentation

14.208.2.1 ProblemDescDB ( )

default constructor

The default constructor: dbRep is NULL in this case. This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

14.208.2.2 ProblemDescDB (ParallelLibrary & *parallel_lib*)

standard constructor

This is the envelope constructor which uses problem_db to build a fully populated db object. It only needs to extract enough data to properly execute get_db(problem_db), since the constructor overloaded with BaseConstructor builds the actual base class data inherited by the derived classes.

References Dakota::abort_handler(), and ProblemDescDB::dbRep.

14.208.2.3 ProblemDescDB (const ProblemDescDB & *db*)

copy constructor

Copy constructor manages sharing of dbRep

14.208.2.4 ∼ProblemDescDB ( )

destructor

dbRep only deleted when its reference count reaches zero.

References Dakota::Dak_pddb.

14.208.2.5 ProblemDescDB (BaseConstructor , ParallelLibrary & *parallel_lib*) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_db() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid the recursion of the base class constructor calling get_db() again). Since the letter IS the representation, its representation pointer is set to NULL.

14.208.3 Member Function Documentation

14.208.3.1 ProblemDescDB operator= (const ProblemDescDB & *db*)

assignment operator

Assignment operator shares the dbRep.

References ProblemDescDB::dbRep.

14.208.3.2 void parse_inputs (ProgramOptions & *prog_opts*, DbCallbackFunctionPtr *callback* = NULL, void * *callback_data* = NULL)

Parses the input file or input string if present and executes callbacks. Does not perform any validation.

DB setup phase 1: parse the input file and execute callback functions if present. Rank 0 only.

DB setup phase 2: optionally insert additional data via late sets. Rank 0 only.

References Dakota::abort_handler(), ProblemDescDB::dbRep, ProblemDescDB::derived_parse_inputs(), ProgramOptions::echo_input(), ProblemDescDB::echo_input_file(), ProgramOptions::input_file(), ProgramOptions::input_string(), ProblemDescDB::parallelLib, ProgramOptions::parser_options(), ProgramOptions::preproc_cmd(), ProgramOptions::preproc_input(), Dakota::pyprepro_input(), Dakota::string_to_tmpfile(), and ParallelLibrary::world_rank().

Referenced by Environment::parse().

14.208.3.3 void check_and_broadcast (const ProgramOptions & *prog_opts*)

performs check_input, broadcast, and post_process, but for now, allowing separate invocation through the public API as well

DB setup phase 3: perform basic checks on keywords counts in current DB state, then sync to all processors.

References ProblemDescDB::broadcast(), ProblemDescDB::check_input(), ProblemDescDB::dbRep, ProblemDescDB::parallelLib, ProblemDescDB::post_process(), and ParallelLibrary::world_rank().

Referenced by LibraryEnvironment::done_modifying_db(), and Environment::parse().

14.208.3.4 void check_input ( )

verifies that there is at least one of each of the required keywords in the dakota input file

NOTE: when using library mode in a parallel application, check_input() should either be called only on worldRank 0, or it should follow a matched send_db_buffer()/receive_db_buffer() pair.

References Dakota::abort_handler(), ParallelLibrary::command_line_post_run_input(), ParallelLibrary::command_line_post_run_output(), ParallelLibrary::command_line_pre_run_input(), ParallelLibrary::command_line_pre_run_output(), ParallelLibrary::command_line_run_input(), ParallelLibrary::command_line_run_output(), ParallelLibrary::command_line_user_modes(), ProblemDescDB::dataInterfaceList, ProblemDescDB::dataMethodList, ProblemDescDB::dataModelList, ProblemDescDB::dataResponsesList, ProblemDescDB::dataVariablesList, ProblemDescDB::dbRep, ProblemDescDB::environmentCntr, ProblemDescDB::parallelLib, and Dakota::strbegins().

Referenced by ProblemDescDB::check_and_broadcast().

14.208.3.5 void post_process ( )

post-processes the (minimal) input specification to assign default variables/responses specification arrays. Used by manage_inputs().

When using library mode in a parallel application, post_process() should be called on all processors following broadcast() of a minimal problem specification.

References ProblemDescDB::dbRep, and ProblemDescDB::derived_post_process().

Referenced by ProblemDescDB::check_and_broadcast().

14.208.3.6 void ** get_voidss (const String & *entry_name*) const

for getting a void**, e.g., &dlLib

This special case involving pointers doesn't use generic lookups

References ProblemDescDB::dbRep.

14.208.3.7 std::shared_ptr< ProblemDescDB > get_db (ParallelLibrary & *parallel_lib*) [private]

Used by the envelope constructor to instantiate the correct letter class.

Initializes dbRep to the appropriate derived type. The standard derived class constructors are invoked.

References Dakota::Dak_pddb.

14.208.3.8 void enforce_unique_ids ( ) [private]

require user-specified block identifiers to be unique

Require string idenfitiers id_* to be unique across all blocks of each type (method, model, variables, interface, responses

For now, this allows duplicate empty ID strings. Would be better to require unique IDs when more than one block of a given type appears in the input file (instead of use-the-last-parsed)

References Dakota::abort_handler(), ProblemDescDB::dataInterfaceList, ProblemDescDB::dataMethodList, ProblemDescDB::dataModelList, ProblemDescDB::dataResponsesList, and ProblemDescDB::dataVariablesList.

Referenced by ProblemDescDB::broadcast().

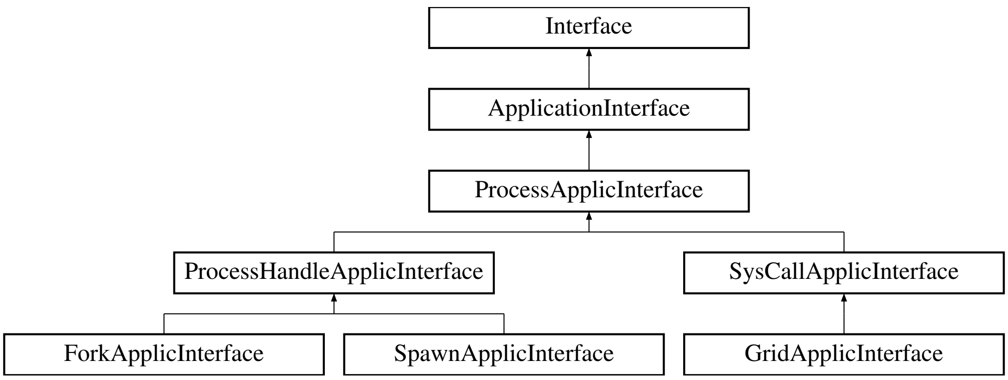
The documentation for this class was generated from the following files:

- ProblemDescDB.hpp
- ProblemDescDB.cpp

14.209 ProcessApplicInterface Class Reference

Derived application interface class that spawns a simulation code using a separate process and communicates with it through files.

Inheritance diagram for ProcessApplicInterface:



Public Member Functions

- ProcessApplicInterface (const ProblemDescDB &problem_db)

constructor

- ∼ProcessApplicInterface ()

    destructor

Protected Member Functions

- void derived_map (const Variables &vars, const ActiveSet &set, Response &response, int fn_eval_id)

    Called by map() and other functions to execute the simulation in synchronous mode. The portion of performing an evaluation that is specific to a derived class.

- void derived_map_asynch (const ParamResponsePair &pair)

    Called by map() and other functions to execute the simulation in asynchronous mode. The portion of performing an asynchronous evaluation that is specific to a derived class.

- void wait_local_evaluations (PRPQueue &prp_queue)

    For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version waits for at least one completion.

- void test_local_evaluations (PRPQueue &prp_queue)

    For asynchronous function evaluations, this method is used to detect completion of jobs and process their results. It provides the processing code that is specific to derived classes. This version is nonblocking and will return without any completions if none are immediately available.

- const StringArray & analysis_drivers () const

    retrieve the analysis drivers specification for application interfaces

- void file_cleanup () const
- void **file_and_workdir_cleanup** (const bfs::path &params_path, const bfs::path &results_path, const bfs::path &workdir_path, const String &tag) const
- void remove_params_results_files (const bfs::path &params_path, const bfs::path &results_path) const

    Remove (potentially autotagged for multiple programs) parameters and results files with passed root names.

- void autotag_files (const bfs::path &params_path, const bfs::path &results_path, const String &eval_id_tag) const

    Utility to automatically tag parameters and results files with passed root names (the files may already need per-program tagging)

- virtual void wait_local_evaluation_sequence (PRPQueue &prp_queue)=0

    version of wait_local_evaluations() managing of set of individual asynchronous evaluations

- virtual void test_local_evaluation_sequence (PRPQueue &prp_queue)=0

    version of test_local_evaluations() managing of set of individual asynchronous evaluations

- virtual void map_bookkeeping (pid_t pid, int fn_eval_id)=0

    bookkeeping of process and evaluation ids for asynchronous maps

- virtual pid_t create_evaluation_process (bool block_flag)=0

    Spawn the evaluation by managing the input filter, analysis drivers, and output filter. Called from derived_map() & derived_map_asynch().

- void wait_local_evaluation_batch (PRPQueue &prp_queue)

    batch version of wait_local_evaluations()

- void test_local_evaluation_batch (PRPQueue &prp_queue)

    batch version of test_local_evaluations()

- void synchronous_local_analyses (int start, int end, int step)

    execute analyses synchronously on the local processor

- void define_filenames (const String &eval_id_tag)

    define modified filenames from user input by handling Unix temp file and optionally tagging with given eval_id_tag

- void write_parameters_files (const Variables &vars, const ActiveSet &set, const Response &response, const int id)

    write the parameters data and response request data to one or more parameters files (using one or more invocations of write_parameters_file()) in either standard or aprepro format

- void read_results_files (Response &response, const int id, const String &eval_id_tag)

    read the response object from one or more results files using full eval_id_tag passed

- bfs::path get_workdir_name ()

    construct a work directory name (tmp or named), with optional tag
- void prepare_process_environment ()

    set PATH, environment variables, and change directory prior to fork/system/spawn
- void reset_process_environment ()

    reset PATH and current directory after system/spawn (workdir case)

Protected Attributes

- bool fileTagFlag

    flags tagging of parameter/results files
- bool fileSaveFlag

    flags retention of parameter/results files
- bool commandLineArgs

    flag indicating use of passing of filenames as command line arguments to the analysis drivers and input/output filters
- bool apreproFlag

    flag indicating use of the APREPRO (the Sandia "A PRE PROcessor" utility) format for parameter files
- unsigned short resultsFileFormat

    results file format
- bool multipleParamsFiles

    flag indicating the need for separate parameters files for multiple analysis drivers
- std::string iFilterName

    the name of the input filter (input_filter user specification)
- std::string oFilterName

    the name of the output filter (output_filter user specification)
- std::vector< String > programNames

    the names of the analysis code programs (analysis_drivers user specification)
- std::string specifiedParamsFileName

    the name of the parameters file from user specification
- std::string paramsFileName

    the parameters file name actually used (modified with tagging or temp files); only valid from define_filenames to write_parameters_files
- std::string paramsFileWritten

    actual, qualified name of the params file written, possibly with workdir
- std::string specifiedResultsFileName

    the name of the results file from user specification
- std::string resultsFileName

    the results file name actually used (modified with tagging or temp files); only valid from define_filenames to write_-parameters_files
- std::string resultsFileWritten

    actual, qualified name of the results file written, possibly with workdir
- std::string fullEvalId

    complete evalIdTag, possibly including hierarchical tagging and final eval id, but not program numbers, for passing to write_parameters_files
- bool allowExistingResults

    by default analysis code interfaces delete results files if they exist; user may override with this flag and we'll try to gather and only fork if needed
- std::map< int, PathTriple > fileNameMap

    Maps function evaluation ID to triples (parameters, results, and workdir) paths used in spawning function evaluations. Workdir will be empty if not created specifically for this eval.
- bool useWorkdir

whether to use a work_directory
- std::string workDirName

    work_directory name, if specified...
- bool dirTag

    whether to tag the working directory
- bool dirSave

    whether dir_save was specified
- bfs::path curWorkdir

    active working directory for this evaluation; valid only from define_filenames to create_evaluation_process
- bfs::path createdDir

    non-empty if created for this eval; valid only from define_filenames to write_parameters_files
- StringArray linkFiles

    template directory (if specified)
- StringArray copyFiles

    template files (if specified)
- bool templateReplace

    whether to replace existing files

Private Member Functions

- void write_parameters_file (const Variables &vars, const ActiveSet &set, const Response &response, const std::string &prog, const std::vector< String > &an_comps, const std::string &params_fname, const bool file_mode_out=true)

    write the variables, active set vector, derivative variables vector, and analysis components to the specified parameters file in either standard or aprepro format
- void read_results_file (Response &response, const bfs::path &path, const int id)

    Open and read the results file at path, properly handling errors.

14.209.1 Detailed Description

Derived application interface class that spawns a simulation code using a separate process and communicates with it through files.

ProcessApplicInterface is subclassed for process handles or file completion testing.

14.209.2 Member Function Documentation

14.209.2.1 void file_cleanup ( ) const [protected], [virtual]

Remove any files and directories still referenced in the fileNameMap

Reimplemented from Interface.

References WorkdirHelper::concat_path(), ProcessApplicInterface::dirSave, ProcessApplicInterface::fileNameMap, ProcessApplicInterface::fileSaveFlag, ProcessApplicInterface::iFilterName, ProcessApplicInterface::multipleParamsFiles, ProcessApplicInterface::programNames, and WorkdirHelper::recursive_remove().

14.209.2.2 void autotag_files (const bfs::path & *params_path,* const bfs::path & *results_path,* const String & *eval_id_tag*) const [protected]

Utility to automatically tag parameters and results files with passed root names (the files may already need per-program tagging)

Move specified params and results files to unique tagged versions when needed

References WorkdirHelper::concat_path(), ProcessApplicInterface::iFilterName, ProcessApplicInterface::multipleParamsFiles, ProcessApplicInterface::oFilterName, Interface::outputLevel, ProcessApplicInterface::programNames, WorkdirHelper::rename(), ProcessApplicInterface::specifiedParamsFileName, ProcessApplicInterface::specifiedResultsFileName, and ApplicationInterface::suppressOutput.

14.209.2.3 void synchronous_local_analyses (int *start*, int *end*, int *step*) [inline], [protected]

execute analyses synchronously on the local processor

Execute analyses synchronously in succession on the local processor (start to end in step increments). Modeled after ApplicationInterface::synchronous_local_evaluations().

References ApplicationInterface::synchronous_local_analysis().

Referenced by ProcessHandleApplicInterface::create_evaluation_process().

14.209.2.4 void prepare_process_environment ( ) [protected]

set PATH, environment variables, and change directory prior to fork/system/spawn

Guidance: environment (PATH, current directory) should be set immediately before Dakota spawns a process and reset immediately afterwards (except fork which never returns)

References WorkdirHelper::change_directory(), ProcessApplicInterface::curWorkdir, Interface::outputLevel, ProcessApplicInterface::paramsFileName, ProcessApplicInterface::resultsFileName, WorkdirHelper::set_environment(), WorkdirHelper::set_preferred_path(), and ProcessApplicInterface::useWorkdir.

Referenced by SpawnApplicInterface::create_analysis_process(), ForkApplicInterface::create_analysis_process(), SysCallApplicInterface::spawn_analysis_to_shell(), SysCallApplicInterface::spawn_evaluation_to_shell(), SysCallApplicInterface::spawn_input_filter_to_shell(), and SysCallApplicInterface::spawn_output_filter_to_shell().

14.209.2.5 void reset_process_environment ( ) [protected]

reset PATH and current directory after system/spawn (workdir case)

Undo anything done prior to spawn

References Interface::outputLevel, WorkdirHelper::reset(), WorkdirHelper::startup_pwd(), and ProcessApplicInterface::useWorkdir.

Referenced by SpawnApplicInterface::create_analysis_process(), ForkApplicInterface::create_analysis_process(), SysCallApplicInterface::spawn_analysis_to_shell(), SysCallApplicInterface::spawn_evaluation_to_shell(), SysCallApplicInterface::spawn_input_filter_to_shell(), and SysCallApplicInterface::spawn_output_filter_to_shell().

14.209.2.6 void read_results_file (Response & *response*, const bfs::path & *path*, const int *id*) [private]

Open and read the results file at path, properly handling errors.

Helper for read_results_files that opens the results file at results_path and reads it, handling various errors/exceptions.

References Dakota::abort_handler(), Response::read(), and ProcessApplicInterface::resultsFileFormat.

Referenced by ProcessApplicInterface::read_results_files().

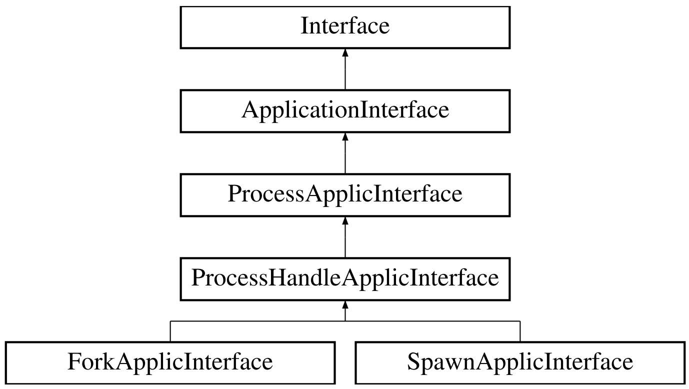
The documentation for this class was generated from the following files:

- ProcessApplicInterface.hpp
- ProcessApplicInterface.cpp

14.210 ProcessHandleApplicInterface Class Reference

Derived application interface class that spawns a simulation code using a separate process, receives a process identifier, and communicates with the spawned process through files.

Inheritance diagram for ProcessHandleApplicInterface:



Public Member Functions

- ProcessHandleApplicInterface (const ProblemDescDB &problem_db)

    constructor
- ∼ProcessHandleApplicInterface ()

    destructor

Protected Member Functions

- int synchronous_local_analysis (int analysis_id)
- void init_communicators_checks (int max_eval_concurrency)
- void set_communicators_checks (int max_eval_concurrency)
- void map_bookkeeping (pid_t pid, int fn_eval_id)

    bookkeeping of process and evaluation ids for asynchronous maps
- pid_t create_evaluation_process (bool block_flag)
- virtual pid_t create_analysis_process (bool block_flag, bool new_group)=0

    spawn a child process for an analysis component within an evaluation
- virtual size_t wait_local_analyses ()=0

    wait for asynchronous analyses on the local processor, completing at least one job
- virtual size_t test_local_analyses_send (int analysis_id)=0

    test for asynchronous analysis completions on the local processor and return results for any completions by sending messages
- virtual void join_evaluation_process_group (bool new_group)

    create (if new_group) and join the process group for asynch evaluations
- virtual void join_analysis_process_group (bool new_group)

    create (if new_group) and join the process group for asynch analyses
- virtual void evaluation_process_group_id (pid_t pgid)

    set evalProcGroupId
- virtual pid_t evaluation_process_group_id () const

    return evalProcGroupId
- virtual void analysis_process_group_id (pid_t pgid)

    set analysisProcGroupId

- virtual pid_t analysis_process_group_id () const

  return analysisProcGroupId
- void process_local_evaluation (PRPQueue &prp_queue, const pid_t pid)

  Common processing code used by {wait,test}_local_evaluations.
- void check_wait (pid_t pid, int status)

  check the exit status of a forked process and abort if an error code was returned
- void asynchronous_local_analyses (int start, int end, int step)

  execute analyses asynchronously on the local processor
- void serve_analyses_asynch ()

  serve the analysis scheduler and execute analysis jobs asynchronously
- void ifilter_argument_list ()

  set argList for execution of the input filter
- void ofilter_argument_list ()

  set argList for execution of the output filter
- void driver_argument_list (int analysis_id)

  set argList for execution of the specified analysis driver
- void create_command_arguments (boost::shared_array< const char * > &av, StringArray &driver_and_args)

  parse argList into argument array av suitable for passing to execvp, appending parameters and results filenames if requested by commandLineArgs

Protected Attributes

- std::map< pid_t, int > evalProcessIdMap

  map of fork process id's to function evaluation id's for asynchronous evaluations
- std::map< pid_t, int > analysisProcessIdMap

  map of fork process id's to analysis job id's for asynchronous analyses
- std::vector< std::string > argList

  *an array of strings for use with execvp(const char *, char * const *). These are converted to an array of const char*'s in fork_program().*

14.210.1 Detailed Description

Derived application interface class that spawns a simulation code using a separate process, receives a process identifier, and communicates with the spawned process through files.

ProcessHandleApplicInterface is subclassed for fork/execvp/waitpid (Unix) and spawnvp (Windows).

14.210.2 Constructor & Destructor Documentation

14.210.2.1 ProcessHandleApplicInterface (const ProblemDescDB & *problem_db*) [inline]

constructor

argList sized 3 for [driver name, input file, output file]

14.210.3 Member Function Documentation

14.210.3.1 int synchronous_local_analysis (int *analysis_id*) [inline], [protected], [virtual]

This code provides the derived function used by ApplicationInterface:: serve_analyses_synch() as well as a convenience function for ProcessHandleApplicInterface::synchronous_local_analyses() below.

Reimplemented from ApplicationInterface.

References ProcessHandleApplicInterface::create_analysis_process(), and ProcessHandleApplicInterface::driver_argument_list().

14.210.3.2 void init_communicators_checks (int *max_eval_concurrency*) [inline], [protected], [virtual]

No derived interface plug-ins, so perform construct-time checks. However, process init issues as warnings since some contexts (e.g., HierarchSurrModel) initialize more configurations than will be used.

Reimplemented from ApplicationInterface.

References ApplicationInterface::check_multiprocessor_analysis(), and ApplicationInterface::check_multiprocessor_asynchronous().

14.210.3.3 void set_communicators_checks (int *max_eval_concurrency*) [inline], [protected], [virtual]

Process run-time issues as hard errors.

Reimplemented from ApplicationInterface.

References Dakota::abort_handler(), ApplicationInterface::check_multiprocessor_analysis(), and ApplicationInterface::check_multiprocessor_asynchronous().

14.210.3.4 pid_t create_evaluation_process (bool *block_flag*) [protected], [virtual]

Manage the input filter, 1 or more analysis programs, and the output filter in blocking or nonblocking mode as governed by block_flag. In the case of a single analysis and no filters, a single fork is performed, while in other cases, an initial fork is reforked multiple times. Called from derived_map() with block_flag == BLOCK and from derived_map_asynch() with block_flag == FALL_THROUGH. Uses create_analysis_process() to spawn individual program components within the function evaluation.

Implements ProcessApplicInterface.

References Dakota::abort_handler(), ProcessHandleApplicInterface::analysis_process_group_id(), ApplicationInterface::analysisServerId, ApplicationInterface::asynchLocalAnalysisConcurrency, ApplicationInterface::asynchLocalAnalysisFlag, ProcessHandleApplicInterface::asynchronous_local_analyses(), ParallelLibrary::barrier_e(), ProcessApplicInterface::commandLineArgs, ProcessHandleApplicInterface::create_analysis_process(), ProcessHandleApplicInterface::driver_argument_list(), ApplicationInterface::eaDedMasterFlag, ApplicationInterface::evalCommRank, ApplicationInterface::evalCommSize, ProcessHandleApplicInterface::evalProcessIdMap, ProcessHandleApplicInterface::evaluation_process_group_id(), ProcessHandleApplicInterface::ifilter_argument_list(), ProcessApplicInterface::iFilterName, ProcessHandleApplicInterface::join_evaluation_process_group(), ApplicationInterface::master_dynamic_schedule_analyses(), ProcessApplicInterface::multipleParamsFiles, ApplicationInterface::numAnalysisDrivers, ApplicationInterface::numAnalysisServers, ProcessHandleApplicInterface::ofilter_argument_list(), ProcessApplicInterface::oFilterName, ApplicationInterface::parallelLib, ProcessApplicInterface::paramsFileName, ProcessApplicInterface::programNames, ProcessApplicInterface::resultsFileName, ProcessHandleApplicInterface::serve_analyses_asynch(), ApplicationInterface::serve_analyses_synch(), Dakota::substitute_params_and_results(), ApplicationInterface::suppressOutput, and ProcessApplicInterface::synchronous_local_analyses().

14.210.3.5 void check_wait (pid_t *pid,* int *status*) [protected]

check the exit status of a forked process and abort if an error code was returned

Check to see if the process terminated abnormally (WIFEXITED(status)==0) or if either execvp or the application returned a status code of -1 (WIFEXITED(status)!=0 && (signed char)WEXITSTATUS(status)==-1). If one of these conditions is detected, output a failure message and abort. Note: the application code should not return a status code of -1 unless an immediate abort of dakota is wanted. If for instance, failure capturing is to be used, the application code should write the word "FAIL" to the appropriate results file and return a status code of 0 through exit().

References Dakota::abort_handler().

Referenced by ForkApplicInterface::create_analysis_process(), SpawnApplicInterface::test_local_analyses_send(), SpawnApplicInterface::test_local_evaluation_sequence(), ForkApplicInterface::wait(), SpawnApplicInterface::wait_-local_analyses(), and SpawnApplicInterface::wait_local_evaluation_sequence().

14.210.3.6 void asynchronous_local_analyses (int *start,* int *end,* int *step*) [protected]

execute analyses asynchronously on the local processor

Schedule analyses asynchronously on the local processor using a dynamic scheduling approach (start to end in step increments). Concurrency is limited by asynchLocalAnalysisConcurrency. Modeled after ApplicationInterface-::asynchronous_local_evaluations(). NOTE: This function should be elevated to ApplicationInterface if and when another derived interface class supports asynchronous local analyses.

References Dakota::abort_handler(), ProcessHandleApplicInterface::analysisProcessIdMap, ApplicationInterface-::asynchLocalAnalysisConcurrency, ProcessHandleApplicInterface::create_analysis_process(), ProcessHandle-ApplicInterface::driver_argument_list(), ApplicationInterface::numAnalysisDrivers, and ProcessHandleApplic-Interface::wait_local_analyses().

Referenced by ProcessHandleApplicInterface::create_evaluation_process().

14.210.3.7 void serve_analyses_asynch ( ) [protected]

serve the analysis scheduler and execute analysis jobs asynchronously

This code runs multiple asynch analyses on each server. It is modeled after ApplicationInterface::serve_evaluations-_asynch(). NOTE: This fn should be elevated to ApplicationInterface if and when another derived interface class supports hybrid analysis parallelism.

References Dakota::abort_handler(), ProcessHandleApplicInterface::analysisProcessIdMap, ApplicationInterface-::asynchLocalAnalysisConcurrency, ProcessHandleApplicInterface::create_analysis_process(), ProcessHandle-ApplicInterface::driver_argument_list(), ParallelLibrary::irecv_ea(), ApplicationInterface::numAnalysisDrivers, ApplicationInterface::parallelLib, ParallelLibrary::recv_ea(), ParallelLibrary::test(), and ProcessHandleApplic-Interface::test_local_analyses_send().

Referenced by ProcessHandleApplicInterface::create_evaluation_process().

14.210.3.8 void create_command_arguments (boost::shared_array$<$ const char $*$ $>$ & *av,* StringArray & *driver_and_args*) [protected]

parse argList into argument array av suitable for passing to execvp, appending parameters and results filenames if requested by commandLineArgs

This function will split the analysis command in argList[0] based on whitespace, but preserve spaces within quoted strings, such that quoted strings can be passed as single command arguments. NOTE: This function allocates memory in av that might be implicitly freed when the child exits (control never returns to caller). driver_and_args needs to be a return argument because av will contain pointers into its c_str()'s when done.

References ProcessHandleApplicInterface::argList, ProcessApplicInterface::commandLineArgs, Dakota::substitute-_params_and_results(), and WorkdirHelper::tokenize_driver().

Referenced by SpawnApplicInterface::create_analysis_process(), and ForkApplicInterface::create_analysis_-process().

The documentation for this class was generated from the following files:

- ProcessHandleApplicInterface.hpp
- ProcessHandleApplicInterface.cpp

14.211 ProgramOptions Class Reference

ProgramOptions stores options whether from the CLH or from library user; initially valid only on worldRank = 0, but then broadcast in ParallelLibrary::push_output_tag()

Public Member Functions

- ProgramOptions ()

  default constructor (needed for default environment ctors and could be used by library clients to late update data)
- ProgramOptions (int world_rank)

  constructor that accepts world rank to help with I/O control; allows default constructed ProgramOptions to get rank in library mode
- ProgramOptions (int argc, char ∗argv[ ], int world_rank)

  standard constructor that uses a CommandLineHandler to parse user options
- const String & input_file () const

  Dakota input file base name (no tag)
- const String & input_string () const

  alternate Dakota input string literal; also set when input is read from stdin
- bool echo_input () const

  is input echo specified?
- bool preproc_input () const

  pre-process input file
- const String & preproc_cmd () const

  pre-processing command, possibly specifying another tool
- const String & parser_options () const

  (deprecated) NIDR parser options
- String output_file () const

  output (user-provided or default) file base name (no tag)
- const String & error_file () const

  error file base name (no tag)
- const String & exit_mode () const

  behavior of abort_handler (throw or exit)
- const String & read_restart_file () const

  restart file base name (no tag)
- size_t stop_restart_evals () const

  eval ID at which to stop reading restart
- String write_restart_file () const

  write retart (user-provided or default) file base name (no tag)
- bool help () const

  is help mode active?
- bool version () const

  is version mode active?
- bool check () const

  is check mode active?
- bool pre_run () const

  is pre-run mode active?
- bool run () const

  is run mode active?
- bool post_run () const

  is post-run mode active?
- bool user_modes () const

are any non-default, user-specified run modes active?

- const String & pre_run_input () const

  filename for pre-run input
- const String & pre_run_output () const

  filename for pre-run output
- const String & run_input () const

  filename for run input
- const String & run_output () const

  filename for run output
- const String & post_run_input () const

  filename for post-run input
- const String & post_run_output () const

  filename for post-run output
- unsigned int pre_run_output_format () const

  tabular format for pre-run output
- unsigned int post_run_input_format () const

  tabular format for post-run input
- bool proceed_to_instantiate () const

  whether steps beyond help/version are requested (instantiation required)
- bool proceed_to_run () const

  Whether steps beyond check are requested.
- bool user_stdout_redirect () const

  whether the user/client code requested a redirect of stdout
- bool user_stderr_redirect () const

  whether the user/client code requested a redirect of stderr
- void world_rank (int world_rank)

  set the world rank to govern early conditional output
- void input_file (const String &in_file)

  set Dakota input file base name (no tag)
- void input_string (const String &in_string)

  set alternate Dakota input string literal
- void echo_input (bool echo_flag)

  set whether to echo input to output
- void preproc_input (bool pp_flag)

  set whether to pre-process input file
- void preproc_cmd (const String &pp_cmd)

  set alternate pre-processing command
- void exit_mode (const String &mode)

  set behavior for abort_handler
- void output_file (const String &out_file)

  set base file name for Dakota output
- void error_file (const String &err_file)

  set base file name for Dakota errors
- void read_restart_file (const String &read_rst)

  set base file name for restart file from which to read
- void stop_restart_evals (size_t stop_rst)

  set eval ID at which to stop reading restart
- void write_restart_file (const String &write_rst)

  set base file name for restart file to write
- void help (bool help_flag)

  set true to print help information and exit

- void version (bool version_flag)

  set true to print version information and exit
- void check (bool check_flag)

  set true to check input and instantiate objects, then exit
- void pre_run (bool pre_run_flag)

  set to enable/disable pre-run phase
- void run (bool run_flag)

  set to enable/disable run phase
- void post_run (bool post_run_flag)

  set to enable/disable post-run phase
- void pre_run_input (const String &pre_run_in)

  Specify the pre-run phase input filename.
- void pre_run_output (const String &pre_run_out)

  Specify the pre-run phase output filename.
- void run_input (const String &run_in)

  Specify the run phase input filename.
- void run_output (const String &run_out)

  Specify the run phase output filename.
- void post_run_input (const String &post_run_in)

  Specify the post-run phase input filename.
- void post_run_output (const String &post_run_out)

  Specify the post-run phase output filename.
- void parse (const ProblemDescDB &problem_db)

  Extract environment options from ProblemDescDB.
- void read (MPIUnpackBuffer &s)

  helper function for reading some class data from MPI buffer
- void write (MPIPackBuffer &s) const

  helper function for writing some class data to MPI buffer

Private Member Functions

- void parse_environment_options ()

  any environment variables affecting global behavior get read here
- void manage_run_modes (const CommandLineHandler &clh)

  retrieve run mode options from the CLH
- void split_filenames (const char *filenames, std::string &input_filename, std::string &output_filename)

  manage pre/run/post filenames
- void validate ()

  verify consistency of user settings (helpful for library mode especially)
- void validate_run_modes ()

  validate user run modes and set userModesFlag
- void set_option (const ProblemDescDB &problem_db, const String &db_name, String &data_member)

  retrieve environment.db_name from the problem db and update data_member, warning if needed

Private Attributes

- int worldRank

  cache the world rank to help with conditional output
- String inputFile

  Dakota input file name, e.g., "dakota.in".
- String inputString

  alternate input means for library clients: input string (mutually exclusive with input file)
- bool echoInput

  whether to echo client's input file at parse
- bool preprocInput

  whether to pre-process input with pyprepro/etc.
- String preprocCmd

  pre-processing command (default pyprepro.py)
- String parserOptions

  Deprecated option for NIDR parser options.
- String exitMode

  Abort or throw on error.
- String outputFile

  Dakota output base file name, e.g., "dakota.out".
- String errorFile

  Dakota error base file name, e.g., "dakota.err".
- String readRestartFile

  e.g., "dakota.old.rst"
- size_t stopRestartEvals

  eval number at which to stop restart read
- String writeRestartFile

  e.g., "dakota.new.rst"
- bool helpFlag

  whether to print help message and exit
- bool versionFlag

  whether to print version message and exit
- bool checkFlag

  flags invocation with command line option -check
- bool preRunFlag

  flags invocation with command line option -pre_run
- bool runFlag

  flags invocation with command line option -run
- bool postRunFlag

  flags invocation with command line option -post_run
- bool userModesFlag

  whether any user run modes are active
- String preRunInput

  filename for pre_run input
- String preRunOutput

  filename for pre_run output
- String runInput

  filename for run input
- String runOutput

  filename for run output
- String postRunInput

filename for post_run input

- String postRunOutput

    filename for post_run output

- unsigned short preRunOutputFormat

    tabular format for pre_run output

- unsigned short postRunInputFormat

    tabular format for post_run input

14.211.1 Detailed Description

ProgramOptions stores options whether from the CLH or from library user; initially valid only on worldRank = 0, but then broadcast in ParallelLibrary::push_output_tag()

14.211.2 Member Function Documentation

14.211.2.1 void split_filenames (const char ∗ *filenames,* std::string & *input_filename,* std::string & *output_filename*) [private]

manage pre/run/post filenames

Tokenize colon-delimited input and output filenames, returns unchanged strings if tokens not found.

Referenced by ProgramOptions::manage_run_modes().

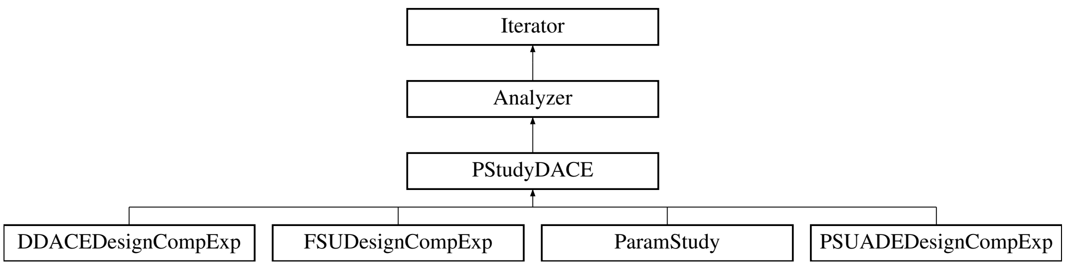
The documentation for this class was generated from the following files:

- ProgramOptions.hpp
- ProgramOptions.cpp

14.212 PStudyDACE Class Reference

Base class for managing common aspects of parameter studies and design of experiments methods.

Inheritance diagram for PStudyDACE:



Public Member Functions

- bool resize ()

    reinitializes iterator based on new variable size

Protected Member Functions

- PStudyDACE (ProblemDescDB &problem_db, Model &model)

constructor

- PStudyDACE (unsigned short method_name, Model &model)

  alternate constructor for instantiations "on the fly"

- ∼PStudyDACE ()

  destructor

- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final iterator results

- void volumetric_quality (int ndim, int num_samples, double ∗sample_points)

  Calculation of volumetric quality measures.

Protected Attributes

- SensAnalysisGlobal pStudyDACESensGlobal

  initialize statistical post processing

- bool volQualityFlag

  flag which specifies evaluation of volumetric quality measures

- bool varBasedDecompFlag

  flag which specifies calculating variance based decomposition sensitivity analysis metrics

Private Attributes

- double chiMeas

  quality measure

- double dMeas

  quality measure

- double hMeas

  quality measure

- double tauMeas

  quality measure

Additional Inherited Members

14.212.1 Detailed Description

Base class for managing common aspects of parameter studies and design of experiments methods.

The PStudyDACE base class manages common data and functions, such as those involving the best solutions located during the parameter set evaluations or the printing of final results.

14.212.2 Member Function Documentation

14.212.2.1 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

References PStudyDACE::chiMeas, Analyzer::compactMode, Model::continuous_variable_labels(), SensAnalysis-Global::correlations_computed(), Model::discrete_int_variable_labels(), Model::discrete_real_variable_labels(), Model::discrete_string_variable_labels(), PStudyDACE::dMeas, PStudyDACE::hMeas, Iterator::iteratedModel, Analyzer::numLSqTerms, Analyzer::numObjFns, SensAnalysisGlobal::print_correlations(), Analyzer::print_-results(), Analyzer::print_sobol_indices(), PStudyDACE::pStudyDACESensGlobal, Model::response_labels(), P-StudyDACE::tauMeas, PStudyDACE::varBasedDecompFlag, and PStudyDACE::volQualityFlag.

14.212.2.2 void volumetric_quality (int *ndim*, int *num_samples*, double ∗ *sample_points*) [protected]

Calculation of volumetric quality measures.

Calculation of volumetric quality measures developed by FSU.

References PStudyDACE::chiMeas, PStudyDACE::dMeas, PStudyDACE::hMeas, and PStudyDACE::tauMeas.

Referenced by FSUDesignCompExp::get_parameter_sets(), and DDACEDesignCompExp::get_parameter_sets().

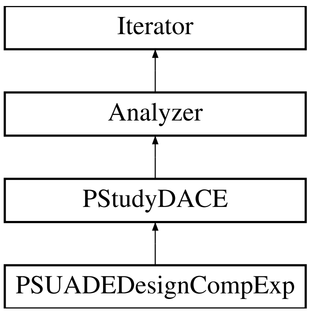
The documentation for this class was generated from the following files:

- DakotaPStudyDACE.hpp
- DakotaPStudyDACE.cpp

14.213 PSUADEDesignCompExp Class Reference

Wrapper class for the PSUADE library.

Inheritance diagram for PSUADEDesignCompExp:



Public Member Functions

- PSUADEDesignCompExp (ProblemDescDB &problem_db, Model &model)

    primary constructor for building a standard DACE iterator
- ∼PSUADEDesignCompExp ()

    destructor
- bool resize ()

    reinitializes iterator based on new variable size

Protected Member Functions

- void pre_run ()

    pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void post_input ()

    read tabular data for post-run mode
- void core_run ()

    core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

- void post_run (std::ostream &s)

    post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/-Responses and perform final analysis phase in a standalone way
- size_t num_samples () const
- void sampling_reset (size_t min_samples, bool all_data_flag, bool stats_flag)

    reset sampling iterator to use at least min_samples
- unsigned short sampling_scheme () const

    return sampling name
- void vary_pattern (bool pattern_flag)

    sets varyPattern in derived classes that support it
- void get_parameter_sets (Model &model)

    Generate one block of numSamples samples (ndim $*$ num_samples), populating allSamples; ParamStudy is the only class that specializes to use allVariables.

Private Member Functions

- void enforce_input_rules ()

    enforce sanity checks/modifications for the user input specification

Private Attributes

- int samplesSpec

    initial specification of number of samples
- size_t numSamples

    current number of samples to be evaluated
- const UShortArray & varPartitionsSpec

    number of partitions in each variable direction
- int numPartitions

    number of partitions to pass to PSUADE (levels = partitions + 1)
- bool allDataFlag

    flag which triggers the update of allVars/allResponses for use by Iterator::all_variables() and Iterator::all_responses()
- size_t numDACERuns

    counter for number of executions for this object
- bool varyPattern

    flag for generating a sequence of seed values within multiple get_parameter_sets() calls so that the sample sets are not repeated, but are still repeatable
- const int seedSpec

    the user seed specification for the random number generator (allows repeatable results)
- int randomSeed

    current seed for the random number generator

Additional Inherited Members

14.213.1 Detailed Description

Wrapper class for the PSUADE library.

The PSUADEDesignCompExp class provides a wrapper for PSUADE, a C++ design of experiments library from Lawrence Livermore National Laboratory. Currently this class only includes the PSUADE Morris One-at-a-time (MOAT) method to uniformly sample the parameter space spanned by the active bounds of the current Model. It returns all generated samples and their corresponding responses as well as the best sample found.

14.213.2 Constructor & Destructor Documentation

14.213.2.1 PSUADEDesignCompExp (ProblemDescDB & *problem_db,* Model & *model*)

primary constructor for building a standard DACE iterator

This constructor is called for a standard iterator built with data from probDescDB.

References Dakota::abort_handler(), Iterator::maxEvalConcurrency, Iterator::method_string(), Iterator::methodName, Analyzer::numDiscreteIntVars, Analyzer::numDiscreteRealVars, Analyzer::numDiscreteStringVars, and PSUADEDesignCompExp::numSamples.

14.213.3 Member Function Documentation

14.213.3.1 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Analyzer.

References PSUADEDesignCompExp::enforce_input_rules(), PSUADEDesignCompExp::get_parameter_sets(), Iterator::iteratedModel, and Analyzer::pre_run().

14.213.3.2 void core_run ( ) [protected], [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Analyzer::evaluate_parameter_sets(), Iterator::iteratedModel, Analyzer::numLSqTerms, and Analyzer::numObjFns.

14.213.3.3 void post_run (std::ostream & *s*) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Analyzer.

References Dakota::abort_handler(), Analyzer::allResponses, Analyzer::allSamples, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), PSUADEDesignCompExp::enforce_input_rules(), Iterator::iteratedModel, Analyzer::numContinuousVars, Analyzer::numFunctions, PSUADEDesignCompExp::numSamples, and Analyzer::post_run().

14.213.3.4 size_t num_samples ( ) const [inline], [protected], [virtual]

Return current number of evaluation points. Since the calculation of samples, collocation points, etc. might be costly, provide a default implementation here that backs out from the maxEvalConcurrency.

Reimplemented from Analyzer.

References PSUADEDesignCompExp::numSamples.

14.213.3.5 void enforce_input_rules ( ) [private]

enforce sanity checks/modifications for the user input specification

Users may input a variety of quantities, but this function must enforce any restrictions imposed by the sampling algorithms.

References Analyzer::numContinuousVars, PSUADEDesignCompExp::numPartitions, PSUADEDesignCompExp::numSamples, and PSUADEDesignCompExp::varPartitionsSpec.

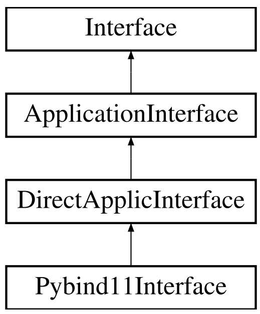
Referenced by PSUADEDesignCompExp::post_input(), PSUADEDesignCompExp::post_run(), and PSUADEDesignCompExp::pre_run().

The documentation for this class was generated from the following files:

- PSUADEDesignCompExp.hpp
- PSUADEDesignCompExp.cpp

14.214 Pybind11Interface Class Reference

Inheritance diagram for Pybind11Interface:



Public Member Functions

- Pybind11Interface (const ProblemDescDB &problem_db)
  constructor
- ∼Pybind11Interface ()
  destructor
- void register_pybind11_callback_fn (py::function callback)
  register a python callback function
- void register_pybind11_callback_fns (const std::map< String, py::function > &callbacks)
  register a collection of python callback functions
- template<typename RetT , class O , class S >
  RetT **copy_array_to_pybind11** (const Teuchos::SerialDenseVector< O, S > &src) const

Protected Member Functions

- void init_communicators_checks (int max_eval_concurrency)
- void set_communicators_checks (int max_eval_concurrency)
- void **initialize_driver** (const String &ac_name)
- virtual int derived_map_ac (const String &ac_name)

execute an analysis code portion of a direct evaluation invocation

- virtual void derived_map_asynch (const ParamResponsePair &pair)

  Python supports batch only, not true asynch (this is no-op)
- virtual void wait_local_evaluations (PRPQueue &prp_queue)

  Python supports batch only, not true asynch (this does the work)
- virtual void test_local_evaluations (PRPQueue &prp_queue)

  Python supports batch only, not true asynch, so this blocks.
- int pybind11_run (const String &ac_name)

  direct interface to Pybind11 via API
- template<typename RetT , class ArrayT , typename T >
  RetT copy_array_to_pybind11 (const ArrayT &src) const

  copy Dakota arrays to pybind11 lists via std::vector<> copy
- template<typename RetT , typename OrdinalType , typename ScalarType >
  RetT copy_array_to_pybind11 (const Teuchos::SerialDenseVector< OrdinalType, ScalarType > &src) const

  specialized copy Dakota arrays to pybind11 lists via std::vector<> copy
- py::dict params_to_dict () const

  Translate Dakota parameters into returned Python dictionary in numpy or array format.
- template<typename T >
  py::dict pack_kwargs () const

  generalized Python dictionary packing to support either lists or numpy arrays
- void unpack_python_response (const ShortArray &asv, const size_t num_derivs, const pybind11::dict &py_response, RealVector &fn_values, RealMatrix &gradients, RealSymMatrixArray &hessians, RealArray &metadata)

  populate values, gradients, Hessians from Python to Dakota
- bool expect_derivative (const ShortArray &asv, const short deriv_type) const

  return true if the passed asv value is requested for any function

Protected Attributes

- bool userNumpyFlag

  whether the user requested numpy data structures in the input file
- bool ownPython

  true if this class created the interpreter instance
- py::function py11CallBack

  callback function for analysis driver
- bool **py11Active**

14.214.1 Detailed Description

Specialization of DirectApplicInterface to link to Python analysis drivers.

14.214.2 Member Function Documentation

14.214.2.1 void init_communicators_checks (int *max_eval_concurrency*) [inline], [protected], [virtual]

Process init issues as warnings since some contexts (e.g., HierarchSurrModel) initialize more configurations than will be used and DirectApplicInterface allows override by derived plug-ins.

Reimplemented from DirectApplicInterface.

14.214.2.2 void set_communicators_checks (int *max_eval_concurrency*) [inline], [protected], [virtual]

Process run-time issues as hard errors.

Reimplemented from DirectApplicInterface.

14.214.2.3 int derived_map_ac (const String & *ac_name*) [protected], [virtual]

execute an analysis code portion of a direct evaluation invocation

Python specialization of derived analysis components.

References ApplicationInterface::analysisServerId, DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, DirectApplicInterface::fnVals, DirectApplicInterface::metaData, Pybind11Interface::params_to_dict(), Pybind11Interface::py11CallBack, and Pybind11Interface::unpack_python_response().

14.214.2.4 void derived_map_asynch (const ParamResponsePair & *pair*) [protected], [virtual]

Python supports batch only, not true asynch (this is no-op)

This is a no-op as all work takes place in wait/test_local_evaluations

Reimplemented from DirectApplicInterface.

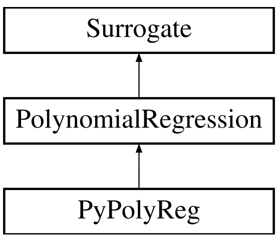
The documentation for this class was generated from the following files:

- Pybind11Interface.hpp
- Pybind11Interface.cpp

14.215 PyPolyReg Class Reference

Extend PolynomialRegression with a new type for Python.

Inheritance diagram for PyPolyReg:



Public Member Functions

- PyPolyReg (const pybind11::dict &pydict)

    ctor that accepts a dictionary
- PyPolyReg (const Eigen::MatrixXd &samples, const Eigen::MatrixXd &response, const pybind11::dict &pydict)

    ctor that accepts a dictionary
- Eigen::MatrixXd value (const Eigen::MatrixXd &eval_points)

    Example workaround for default Eigen pass-by-copy semantics.

Additional Inherited Members

14.215.1 Detailed Description

Extend PolynomialRegression with a new type for Python.

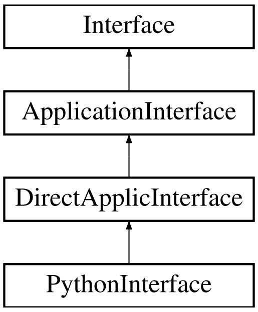
Explore idea of extension as a way to specialize constructors. Permits mapping datatypes for any member functions or constructors that differ, while leaving most untouched. Downside is requires new class for each surrogates class.

The documentation for this class was generated from the following file:

- surrogates_python.cpp

14.216 PythonInterface Class Reference

Inheritance diagram for PythonInterface:



Public Member Functions

- PythonInterface (const ProblemDescDB &problem_db)

  constructor
- ∼PythonInterface ()

  destructor

Protected Member Functions

- virtual int derived_map_ac (const String &ac_name)

  execute an analysis code portion of a direct evaluation invocation
- int python_run (const String &ac_name)

  direct interface to Python via API, BMA 07/02/07
- template<class ArrayT , class Size >
  bool python_convert_int (const ArrayT &src, Size size, PyObject ∗∗dst)

  convert arrays of integer types to Python list or numpy array
- bool python_convert (const RealVector &src, PyObject ∗∗dst)

  convert RealVector to Python list or numpy array
- bool python_convert (const RealVector &c_src, const IntVector &di_src, const RealVector &dr_src, PyObject ∗∗dst)

  convert RealVector + IntVector + RealVector to Python mixed list or numpy double array
- template<class StringArrayT >
  bool python_convert_strlist (const StringArrayT &src, PyObject ∗∗dst)

  convert labels

- bool python_convert (const StringMultiArray &c_src, const StringMultiArray &di_src, const StringMultiArray &dr_src, PyObject ∗∗dst)

    convert all labels to single list
- bool python_convert (PyObject ∗pyv, RealVector &rv, const int &dim)

    convert python [list of int or float] or [numpy array of double] to RealVector (for fns)
- bool python_convert (PyObject ∗pyv, double ∗rv, const int &dim)

    convert python [list of int or float] or [numpy array of double] to double[], for use as helper in converting gradients
- bool python_convert (PyObject ∗pym, RealMatrix &rm)

    convert python [list of lists of int or float] or [numpy array of dbl] to RealMatrix (for gradients)
- bool python_convert (PyObject ∗pym, RealSymMatrix &rm)

    convert python [list of lists of int or float] or [numpy array of dbl] to RealMatrix (used as helper in Hessian conversion)
- bool python_convert (PyObject ∗pyma, RealSymMatrixArray &rma)

    convert python [list of lists of lists of int or float] or [numpy array of double] to RealSymMatrixArray (for Hessians)

Protected Attributes

- bool userNumpyFlag

    whether the user requested numpy data structures in the input file
- bool ownPython

    true if this class created the interpreter instance

14.216.1 Detailed Description

Specialization of DirectApplicInterface to link to Python analysis drivers. Includes convenience functions to map data to/from Python

14.216.2 Member Function Documentation

14.216.2.1 int derived_map_ac (const String & *ac_name*) [protected], [virtual]

execute an analysis code portion of a direct evaluation invocation

Python specialization of derived analysis components.

References ApplicationInterface::analysisServerId, and PythonInterface::python_run().

14.216.2.2 bool python_convert_int (const ArrayT & *src,* Size *sz,* PyObject ∗∗ *dst*) [protected]

convert arrays of integer types to Python list or numpy array

convert all integer array types including IntVector, ShortArray, and SizetArray to Python list of ints or numpy array of ints

References PythonInterface::userNumpyFlag.

Referenced by PythonInterface::python_run().

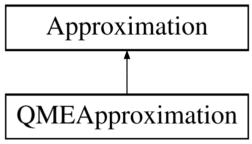
The documentation for this class was generated from the following files:

- PythonInterface.hpp
- PythonInterface.cpp

14.217 QMEApproximation Class Reference

Derived approximation class for QMEA Quadratic Multipoint Exponential Approximation (a multipoint approximation).

Inheritance diagram for QMEApproximation:



Public Member Functions

- QMEApproximation ()

  default constructor
- QMEApproximation (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

  standard constructor
- QMEApproximation (const SharedApproxData &shared_data)

  alternate constructor
- ∼QMEApproximation ()

  destructor

Protected Member Functions

- int min_coefficients () const

  return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- void build ()

  builds the approximation from scratch
- Real value (const Variables &vars)

  retrieve the approximate function value for a given parameter vector
- const RealVector & gradient (const Variables &vars)

  retrieve the approximate function gradient for a given parameter vector
- void clear_current_active_data ()

Private Member Functions

- void find_scaled_coefficients ()

  compute TANA coefficients based on scaled inputs
- void offset (const RealVector &x, RealVector &s)

  based on minX, apply offset scaling to x to define s
- Real **apxfn_value** (const RealVector &)

Private Attributes

- RealVector pExp

  vector of exponent values
- RealVector minX

vector of minimum parameter values used in scaling
- RealVector scX1

  vector of scaled x1 values
- RealVector scX2

  vector of scaled x2 values
- Real H

  the scalar Hessian value in the TANA-3 approximation
- RealVector beta

  vector of QMEA reduced space diagonal Hessian coefficients
- RealMatrix G_reduced_xfm

  Grahm-Schmidt orthonormal reduced subspace transformation.
- size_t numUsed

  number of previous data points used (size of reduced subspace)
- size_t currGradIndex

  index of current expansion point with gradients
- size_t prevGradIndex

  index of most recent previous point with gradients

Additional Inherited Members

14.217.1 Detailed Description

Derived approximation class for QMEA Quadratic Multipoint Exponential Approximation (a multipoint approximation).

The QMEApproximation class provides a multipoint approximation based on matching value and gradient data from multiple points (typically the current and previous iterates) in parameter space. It forms an exponential approximation in terms of intervening variables.

14.217.2 Member Function Documentation

14.217.2.1 void build ( ) [protected], [virtual]

builds the approximation from scratch

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

References Dakota::abort_handler(), Approximation::approxData, Approximation::build(), QMEApproximation::currGradIndex, QMEApproximation::find_scaled_coefficients(), Dakota::length(), QMEApproximation::minX, QMEApproximation::pExp, QMEApproximation::prevGradIndex, and Approximation::sharedDataRep.

14.217.2.2 void clear_current_active_data ( ) [inline], [protected], [virtual]

Redefine default implementation to support history mechanism.

Reimplemented from Approximation.

References Approximation::approxData, QMEApproximation::currGradIndex, QMEApproximation::prevGradIndex, and Approximation::sharedDataRep.

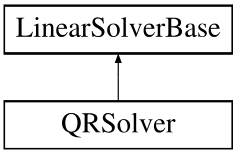
The documentation for this class was generated from the following files:

- QMEApproximation.hpp
- QMEApproximation.cpp

14.218 QRSolver Class Reference

The QRSolver class solves the linear least squares problem with a QR decomposition.

Inheritance diagram for QRSolver:



Public Member Functions

- QRSolver ()

  Constructor.
- ∼QRSolver ()

  Destructor.
- bool is_factorized () const override

  Query to determine if the matrix of the solver has been factored.
- void factorize (const MatrixXd &A) override

  Perform the matrix factorization for the linear solver matrix.
- void solve (const MatrixXd &A, const MatrixXd &b, MatrixXd &x) override

  Find the solution to $(A^{\wedge}T*A)x = A^{\wedge}T*b$ *.*
- void solve (const MatrixXd &b, MatrixXd &x) override

  Find a solution to $(A^{\wedge}T*A)x = A^{\wedge}T*b$ *when A is already factorized.*

Private Attributes

- std::shared_ptr
  < Eigen::ColPivHouseholderQR
  < MatrixXd > > **QR_Ptr**

Additional Inherited Members

14.218.1 Detailed Description

The QRSolver class solves the linear least squares problem with a QR decomposition.

14.218.2 Member Function Documentation

14.218.2.1 void factorize (const MatrixXd & *A*) [override], [virtual]

Perform the matrix factorization for the linear solver matrix.

Parameters

in	*A*	The incoming matrix to factorize.

Reimplemented from LinearSolverBase.

Referenced by QRSolver::solve().

14.218.2.2 void solve (const MatrixXd & *A*, const MatrixXd & *b*, MatrixXd & *x*) [override], [virtual]

Find the solution to (A^T*A)x = A^T*b .

Parameters

in	*A*	The matrix for the QR decomposition.
in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented from LinearSolverBase.

References QRSolver::factorize().

14.218.2.3 void solve (const MatrixXd & *b*, MatrixXd & *x*) [override], [virtual]

Find a solution to (A^T∗A)x = A^T∗b when A is already factorized.

Parameters

in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented from LinearSolverBase.

The documentation for this class was generated from the following files:

- UtilLinearSolvers.hpp
- UtilLinearSolvers.cpp

14.219 QuesoJointPdf< V, M > Class Template Reference

Dakota specialization of QUESO generic joint PDF.

Inherits BaseJointPdf< V, M >.

Public Member Functions

- QuesoJointPdf (const char ∗prefix, const QUESO::VectorSet< V, M > &domainSet, NonDQUESOBayesCalibration ∗nond_queso_ptr)

  Default constructor.
- virtual ∼QuesoJointPdf ()

  Destructor.
- double actualValue (const V &domainVector, const V ∗domainDirection, V ∗gradVector, M ∗hessianMatrix, V ∗hessianEffect) const

  Actual value of the PDF (scalar function).
- double lnValue (const V &domainVector, const V ∗domainDirection, V ∗gradVector, M ∗hessianMatrix, V ∗hessianEffect) const

  Logarithm of the value of the function.
- double computeLogOfNormalizationFactor (unsigned int numSamples, bool m_logOfNormalizationFactor) const

  Computes the logarithm of the normalization factor.
- void distributionMean (V &meanVector) const

  Mean value of underlying random variable.
- void distributionVariance (M &covMatrix) const

  Covariance of the underlying random variable.

Private Attributes

- NonDQUESOBayesCalibration ∗ nonDQUESOInstance

  pointer to QUESO instance for PDF evaluation callbacks

14.219.1 Detailed Description

template<class V, class M>class Dakota::QuesoJointPdf< V, M >

Dakota specialization of QUESO generic joint PDF.

14.219.2 Constructor & Destructor Documentation

14.219.2.1 QuesoJointPdf (const char * *prefix*, const QUESO::VectorSet< V, M > & *domainSet*, NonDQUESOBayesCalibration * *nond_queso_ptr*)

Default constructor.

Instantiates an object of the class, i.e. a scalar function, given a prefix and its domain.

14.219.3 Member Function Documentation

14.219.3.1 void distributionMean (V & *meanVector*) const

Mean value of underlying random variable.

Assumes meanVector is sized

14.219.3.2 void distributionVariance (M & *covMatrix*) const

Covariance of the underlying random variable.

Assumes covMatrix is sized

The documentation for this class was generated from the following files:

- QUESOImpl.hpp
- QUESOImpl.cpp

14.220 QuesoVectorRV< V, M > Class Template Reference

Dakota specialization of QUESO vector-valued random variable.

Inherits BaseVectorRV< V, M >.

Public Member Functions

- QuesoVectorRV (const char *prefix, const QUESO::VectorSet< V, M > &imageSet, NonDQUESOBayesCalibration *nond_queso_ptr)

  Default constructor.
- virtual ~QuesoVectorRV ()

  Virtual destructor.
- void print (std::ostream &os) const

  TODO: Prints the vector RV (required pure virtual).

14.220.1 Detailed Description

template<class V, class M>class Dakota::QuesoVectorRV< V, M >

Dakota specialization of QUESO vector-valued random variable.

14.220.2 Constructor & Destructor Documentation

14.220.2.1 QuesoVectorRV (const char * *prefix*, const QUESO::VectorSet< V, M > & *imageSet*, NonDQUESOBayesCalibration * *nond_queso_ptr*)

Default constructor.

Constructs a generic queso vector RV, given a prefix and the image set of the vector RV.

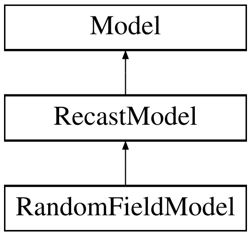
The documentation for this class was generated from the following files:

- QUESOImpl.hpp
- QUESOImpl.cpp

14.221 RandomFieldModel Class Reference

Random field model, capable of generating and then forward propagating.

Inheritance diagram for RandomFieldModel:



Public Member Functions

- RandomFieldModel (ProblemDescDB &problem_db)

  Problem database constructor.
- ∼RandomFieldModel ()

  destructor
- bool initialize_mapping (ParLevLIter pl_iter)

  for KL models, the model is augmented with the random coeffs of the KL
- bool resize_pending () const

  return true if a potential resize is still pending, such that sizing-based initialization should be deferred

Protected Member Functions

- void assign_instance ()

  assign static pointer instance to this for use in static transformation functions
- Model get_sub_model (ProblemDescDB &problem_db)

  retrieve the sub-Model from the DB to pass up the constructor chain
- void init_dace_iterator (ProblemDescDB &problem_db)

initialize the RF-generating sampler
- void validate_inputs ()

  validate the build controls and set defaults
- void get_field_data ()

  Source data generation: get the field data either from file or simulation by running the DACE Iterator. Populates rfBuildData.
- void identify_field_model ()

  Generate field representation: generate a KL or PCA/GP.
- void rf_suite_identify_field_model ()

  Generate field representation: utilize RF Suite.
- void initialize_recast ()

  Initialize the base class RecastModel with reduced space variable sizes.
- SizetArray variables_resize ()

  Create a variables components totals array with the reduced space size for continuous variables.
- void initialize_rf_coeffs ()

  For KL models, augment the subModel's uncertain variables with additional N(0,1) variables; set up mvDist for the N(0,1)'s.
- void derived_evaluate (const ActiveSet &set)

  generate a random field realization, then evaluate the submodel
- void derived_evaluate_nowait (const ActiveSet &set)

  generate a random field realization, then evaluate the submodel (asynch)
- void generate_kl_realization ()

  generate a KL realization and write to file
- void generate_pca_gp_realization ()

  generate a PCA/GP realization and write to file
- void write_field (const RealVector &field_prediction)

  write a field realization to console and file

Static Protected Member Functions

- static void vars_mapping (const Variables &recast_xi_vars, Variables &sub_model_x_vars)

  map the active continuous recast variables to the active submodel variables (linear transformation)
- static void set_mapping (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model-_set)

  map the inbound ActiveSet to the sub-model (map derivative variables)

Protected Attributes

- String rfDataFilename

  name of the data file with RF build data
- size_t numObservations

  rows of data matrix
- IntVector fieldLengths

  column partitions of data matrix
- RealMatrix rfBuildData

  data matrix with realizations of the random field to approximate
- RealMatrix rfBuildVars

  matrix of samples used to build the RF data
- Iterator daceIterator

  String dataDirectoryBasename;.
- unsigned short expansionForm

unsigned short analyticCovForm;
- unsigned short covarianceForm

  form of the analytic covariance function
- int requestedReducedRank

  current approximation of system rank
- Real percentVariance

  fraction of energy to capture
- int actualReducedRank

  command to run RF Suite
- ReducedBasis rfBasis

  reduced basis representation (for KL or PCA case)
- int fieldRealizationId

  counter for RF Suite
- std::vector< Approximation > gpApproximations

  approximate models used to map the uncertain vars through the PCA approx

Static Protected Attributes

- static RandomFieldModel * rfmInstance

  static pointer to this class for use in static callbacks

Additional Inherited Members

14.221.1 Detailed Description

Random field model, capable of generating and then forward propagating.

Specialization of a RecastModel that optionally identifies an approximate random field model during build phase and creates a RecastModel capable of performing forward UQ including the field and auxialliary uncertain variables reduced space. This RandomFieldModel wraps the random field propagation model (not the RF-generating model)

14.221.2 Member Function Documentation

14.221.2.1 bool initialize_mapping (ParLevLIter *pl_iter*) [virtual]

for KL models, the model is augmented with the random coeffs of the KL

May eventually take on init_comms and related operations. Also may want ide of build/update like DataFitSurrModel, eventually.

Reimplemented from Model.

References RandomFieldModel::covarianceForm, Model::estimate_message_lengths(), RandomFieldModel::expansionForm, RandomFieldModel::fieldRealizationId, RandomFieldModel::get_field_data(), RandomFieldModel::identify_field_model(), RecastModel::initialize_mapping(), RandomFieldModel::initialize_recast(), RandomFieldModel::initialize_rf_coeffs(), and RandomFieldModel::rf_suite_identify_field_model().

14.221.2.2 void get_field_data ( ) [protected]

Source data generation: get the field data either from file or simulation by running the DACE Iterator. Populates rfBuildData.

Populate rfBuildData

References Iterator::all_responses(), Iterator::all_samples(), Dakota::copy_data(), Model::cv(), RandomFieldModel::daceIterator, RandomFieldModel::expansionForm, Iterator::is_null(), Iterator::num_samples(), Model::numFns, Dakota::read_sized_data(), RandomFieldModel::rfBuildData, RandomFieldModel::rfBuildVars, Iterator::run(), and RecastModel::subModel.

Referenced by RandomFieldModel::initialize_mapping().

14.221.2.3 void rf_suite_identify_field_model ( ) [protected]

Generate field representation: utilize RF Suite.

Alternative to below function when using RFSuite.

References RandomFieldModel::actualReducedRank, and RandomFieldModel::requestedReducedRank.

Referenced by RandomFieldModel::initialize_mapping().

14.221.2.4 void initialize_recast ( ) [protected]

Initialize the base class RecastModel with reduced space variable sizes.

Initialize the recast model to augment the uncertain variables with actualReducedRank additional N(0,1) variables, with no response function mapping (for now).

References RandomFieldModel::actualReducedRank, Model::continuous_variable_types(), Model::current_-response(), Model::cv(), Model::div(), Model::drv(), Model::dsv(), Response::function_gradients(), Response-::function_hessians(), RecastModel::init_maps(), RecastModel::init_sizes(), Model::num_nonlinear_ineq_-constraints(), Model::num_primary_fns(), Model::num_secondary_fns(), Model::numFns, RandomFieldModel-::set_mapping(), RecastModel::subModel, RandomFieldModel::variables_resize(), and RandomFieldModel::vars_-mapping().

Referenced by RandomFieldModel::initialize_mapping().

14.221.2.5 SizetArray variables_resize ( ) [protected]

Create a variables components totals array with the reduced space size for continuous variables.

Create a variables components totals array with the reduced space size for continuous variables TODO: augment normal uncVars for KL case.

References RandomFieldModel::actualReducedRank, SharedVariablesData::components_totals(), Model::current-_variables(), RandomFieldModel::expansionForm, Variables::shared_data(), RecastModel::subModel, and Dakota-::svd().

Referenced by RandomFieldModel::initialize_recast().

14.221.2.6 void initialize_rf_coeffs ( ) [protected]

For KL models, augment the subModel's uncertain variables with additional N(0,1) variables; set up mvDist for the N(0,1)'s.

Initialzie the aleatory dist params for the KL coeffs

References RandomFieldModel::actualReducedRank, Variables::continuous_variable_label(), Model::continuous_-variable_labels(), Model::currentVariables, RandomFieldModel::expansionForm, Model::multivariate_distribution(), Model::mvDist, and RecastModel::subModel.

Referenced by RandomFieldModel::initialize_mapping().

14.221.2.7 void vars_mapping (const Variables & *recast_xi_vars,* Variables & *sub_model_x_vars*) [static], [protected]

map the active continuous recast variables to the active submodel variables (linear transformation) map the active continuous recast variables to the active submodel variables

References Variables::active_variables(), RandomFieldModel::actualReducedRank, Model::continuous_variable_types(), Variables::continuous_variables(), Model::cv(), Variables::discrete_int_variables(), Model::discrete_int_variables(), Variables::discrete_real_variables(), Model::discrete_real_variables(), Variables::discrete_string_variables(), Model::discrete_string_variables(), RandomFieldModel::expansionForm, RandomFieldModel::rfmInstance, and RecastModel::subModel.

Referenced by RandomFieldModel::initialize_recast().

14.221.3 Member Data Documentation

14.221.3.1 Iterator daceIterator [protected]

String dataDirectoryBasename;.

DACE Iterator to evaluate the RF generating model

Referenced by RandomFieldModel::get_field_data(), RandomFieldModel::init_dace_iterator(), and RandomFieldModel::validate_inputs().

14.221.3.2 unsigned short expansionForm [protected]

unsigned short analyticCovForm;

form of the RF representation (KL, PCA, ICA)

Referenced by RandomFieldModel::derived_evaluate(), RandomFieldModel::derived_evaluate_nowait(), RandomFieldModel::get_field_data(), RandomFieldModel::identify_field_model(), RandomFieldModel::initialize_mapping(), RandomFieldModel::initialize_rf_coeffs(), RandomFieldModel::resize_pending(), RandomFieldModel::variables_resize(), and RandomFieldModel::vars_mapping().

14.221.3.3 int actualReducedRank [protected]

command to run RF Suite

number of bases retained in decomposition

Referenced by RandomFieldModel::generate_kl_realization(), RandomFieldModel::generate_pca_gp_realization(), RandomFieldModel::identify_field_model(), RandomFieldModel::initialize_recast(), RandomFieldModel::initialize_rf_coeffs(), RandomFieldModel::rf_suite_identify_field_model(), RandomFieldModel::variables_resize(), and RandomFieldModel::vars_mapping().

14.221.3.4 RandomFieldModel * rfmInstance [static], [protected]

static pointer to this class for use in static callbacks

initialization of static needed by RecastModel

Referenced by RandomFieldModel::assign_instance(), and RandomFieldModel::vars_mapping().

The documentation for this class was generated from the following files:

- RandomFieldModel.hpp
- RandomFieldModel.cpp

14.222 RealScale Struct Reference

Data structure for storing real-valued dimension scale.

Public Member Functions

- RealScale (const std::string &label, const RealVector &in_items, ScaleScope scope=ScaleScope::UNSHARED)

  Constructor that takes a RealVector.
- RealScale (const std::string &label, const RealArray &in_items, ScaleScope scope=ScaleScope::UNSHARED)

  Constructor that takes a RealArray.
- RealScale (const std::string &label, const Real ∗in_items, const int len, ScaleScope scope=ScaleScope::UNSHARED)

  Constructor that takes a pointer to Real and length.
- RealScale (const std::string &in_label, std::initializer_list< Real > in_items, ScaleScope in_scope=ScaleScope::UNSHARED)

  Constructor that takes an initializer_list.
- RealScale (const std::string &in_label, const RealVectorArray &in_items, ScaleScope in_scope=ScaleScope::UNSHARED)

  Constructor that takes a RealVectorArray.

Public Attributes

- std::string **label**
- ScaleScope **scope**
- RealVector **items**
- int numCols

  Number of columns; equals length of scale when 1D.
- bool isMatrix

  2d or 1d?

14.222.1 Detailed Description

Data structure for storing real-valued dimension scale.

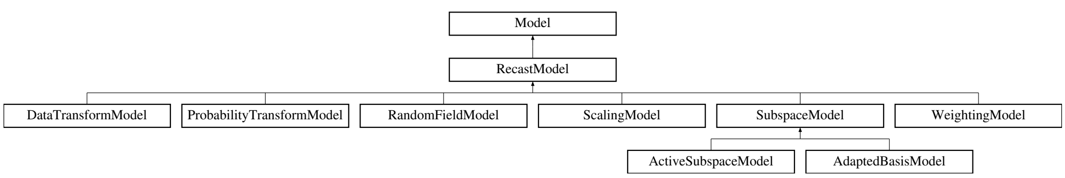
The documentation for this struct was generated from the following file:

- dakota_results_types.hpp

14.223 RecastModel Class Reference

Derived model class which provides a thin wrapper around a sub-model in order to recast the form of its inputs and/or outputs.

Inheritance diagram for RecastModel:



Public Member Functions

- RecastModel (const Model &sub_model, const Sizet2DArray &vars_map_indices, const SizetArray &vars-_comps_total, const BitArray &all_relax_di, const BitArray &all_relax_dr, bool nonlinear_vars_mapping, void(∗variables_map)(const Variables &recast_vars, Variables &sub_model_vars), void(∗set_map)(const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set), const Sizet2DArray &primary_resp_map_indices, const Sizet2DArray &secondary_resp_map_indices, size_t recast_secondary-_offset, short recast_resp_order, const BoolDequeArray &nonlinear_resp_mapping, void(∗primary_resp-_map)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_-response, Response &recast_response), void(∗secondary_resp_map)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response))

    standard (full) constructor; assumes provided sizes and map functions are final and constructs all member data
- RecastModel (const Model &sub_model, const SizetArray &vars_comps_totals, const BitArray &all_relax_-di, const BitArray &all_relax_dr, size_t num_recast_primary_fns, size_t num_recast_secondary_fns, size_t recast_secondary_offset, short recast_resp_order)

    alternate constructor; uses provided sizes to construct Variables, Response and Constraints so Model can be passed to an Iterator; requires subsequent init_maps() call.
- RecastModel (ProblemDescDB &problem_db, const Model &sub_model)

    Problem DB-based ctor, e.g., for use in subspace model; assumes mappings to be initialized later; only initializes based on sub-model.
- RecastModel (const Model &sub_model)

    lightest constructor used when transform sizes aren't known at construct time; doesn't initialize variables and responses, so this Model can't be used to construct an Iterator; requires subsequent init_sizes() and init_maps() calls.
- ∼RecastModel ()

    destructor
- void init_sizes (const SizetArray &vars_comps_totals, const BitArray &all_relax_di, const BitArray &all_relax_-dr, size_t num_recast_primary_fns, size_t num_recast_secondary_fns, size_t recast_secondary_offset, short recast_resp_order)

    update recast sizes and size Variables and Response members after alternate construction
- void init_maps (const Sizet2DArray &vars_map_indices, bool nonlinear_vars_mapping, void(∗variables_-map)(const Variables &recast_vars, Variables &sub_model_vars), void(∗set_map)(const Variables &recast-_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set), const Sizet2DArray &primary_resp_map-_indices, const Sizet2DArray &secondary_resp_map_indices, const BoolDequeArray &nonlinear_resp_-mapping, void(∗primary_resp_map)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response), void(∗secondary_resp_map)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response))

    initialize recast indices and map callbacks after alternate construction
- void inverse_mappings (void(∗inv_vars_map)(const Variables &sub_model_vars, Variables &recast_vars), void(∗inv_set_map)(const Variables &sub_model_vars, const ActiveSet &sub_model_set, ActiveSet &recast-_set), void(∗inv_pri_resp_map)(const Variables &recast_vars, const Variables &sub_model_vars, const Response &recast_resp, Response &sub_model_resp), void(∗inv_sec_resp_map)(const Variables &recast_-vars, const Variables &sub_model_vars, const Response &recast_resp, Response &sub_model_resp))

    provide optional inverse mappings
- void transform_variables (const Variables &recast_vars, Variables &sub_model_vars)

    perform transformation of Variables (recast –> sub-model)
- void transform_set (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)

    into sub_model_set for use with subModel.
- void transform_response (const Variables &recast_vars, const Variables &sub_model_vars, const Response &sub_model_resp, Response &recast_resp)

    perform transformation of Response (sub-model –> recast)
- void transform_response_map (const IntResponseMap &old_resp_map, IntResponseMap &new_resp_map)

    invoke transform_response() on each response within old_resp_map to create new_resp_map
- void inverse_transform_variables (const Variables &sub_model_vars, Variables &recast_vars)

    perform inverse transformation of Variables (sub-model –> recast)

- void inverse_transform_set (const Variables &sub_model_vars, const ActiveSet &sub_model_set, ActiveSet &recast_set)

  into sub_model_set for use with subModel.

- void inverse_transform_response (const Variables &sub_model_vars, const Variables &recast_vars, const Response &recast_resp, Response &sub_model_resp)

  perform inverse transformation of Response (recast –> sub-model)

- void submodel_supports_derivative_estimation (bool sed_flag)

  override the submodel's derivative estimation behavior

- String root_model_id ()

  Return the model ID of the "innermost" model. For all derived Models except RecastModels, return modelId. The RecastModel override returns the root_model_id() of the subModel.

- ActiveSet **default_active_set** ()
- void declare_sources ()

  Declare a model's sources to the evaluationsDB.

- bool nonlinear_variables_mapping () const

  return nonlinearVarsMapping

Protected Member Functions

- Pecos::ProbabilityTransformation & probability_transformation ()

  return probability transformation employed by the Model (forwarded along to ProbabilityTransformModel recasting)

- bool initialize_mapping (ParLevLIter pl_iter)

  Perform any global updates prior to individual evaluate() calls; returns true if the variables size has changed.

- bool finalize_mapping ()

  restore state in preparation for next initialization; returns true if the variables size has changed

- void nested_variable_mappings (const SizetArray &c_index1, const SizetArray &di_index1, const SizetArray &ds_index1, const SizetArray &dr_index1, const ShortArray &c_target2, const ShortArray &di_target2, const ShortArray &ds_target2, const ShortArray &dr_target2)

  set primaryA{C,DI,DS,DR}VarMapIndices, secondaryA{C,DI,DS,DR}VarMapTargets (coming from a higher-level NestedModel context to inform derivative est.)

- const SizetArray & nested_acv1_indices () const

  return primaryACVarMapIndices

- const ShortArray & nested_acv2_targets () const

  return secondaryACVarMapTargets

- short query_distribution_parameter_derivatives () const

  calculate and return derivative composition of final results w.r.t. distribution parameters (none, all, or mixed)

- void activate_distribution_parameter_derivatives ()

  activate derivative setting w.r.t. distribution parameters

- void deactivate_distribution_parameter_derivatives ()

  deactivate derivative setting w.r.t. distribution parameters

- void trans_grad_X_to_U (const RealVector &fn_grad_x, RealVector &fn_grad_u, const RealVector &x_vars)

  transform x-space gradient vector to u-space

- void trans_grad_U_to_X (const RealVector &fn_grad_u, RealVector &fn_grad_x, const RealVector &x_vars)

  transform u-space gradient vector to x-space

- void trans_grad_X_to_S (const RealVector &fn_grad_x, RealVector &fn_grad_s, const RealVector &x_vars)

  transform x-space gradient vector to gradient with respect to inserted distribution parameters

- void trans_hess_X_to_U (const RealSymMatrix &fn_hess_x, RealSymMatrix &fn_hess_u, const RealVector &x_vars, const RealVector &fn_grad_x)

  transform x-space Hessian matrix to u-space

- size_t qoi () const

  return number of unique response functions (managing any aggregations)

- void derived_evaluate (const ActiveSet &set)

    portion of evaluate() specific to RecastModel (forward to subModel.evaluate())
- void derived_evaluate_nowait (const ActiveSet &set)

    portion of evaluate_nowait() specific to RecastModel (forward to subModel.evaluate_nowait())
- const IntResponseMap & derived_synchronize ()

    portion of synchronize() specific to RecastModel (forward to subModel.synchronize())
- const IntResponseMap & derived_synchronize_nowait ()

    portion of synchronize_nowait() specific to RecastModel (forward to subModel.synchronize_nowait())
- Iterator & subordinate_iterator ()

    return sub-iterator, if present, within subModel
- Model & subordinate_model ()

    return subModel
- void active_model_key (const Pecos::ActiveKey &key)

    set key in subModel
- const Pecos::ActiveKey & active_model_key () const

    return key from subModel
- void clear_model_keys ()

    remove keys in subModel
- Model & surrogate_model (size_t i=_NPOS)

    return surrogate model, if present, within subModel
- const Model & surrogate_model (size_t i=_NPOS) const

    return surrogate model, if present, within subModel
- Model & truth_model ()

    return truth model, if present, within subModel
- const Model & truth_model () const

    return truth model, if present, within subModel
- void derived_subordinate_models (ModelList &ml, bool recurse_flag)

    add subModel to list and recurse into subModel
- void resize_from_subordinate_model (size_t depth=SZ_MAX)

    pass request to subModel if recursing and then resize from its results
- void update_from_subordinate_model (size_t depth=SZ_MAX)

    pass request to subModel if recursing and then update from its results
- Interface & derived_interface ()

    return subModel interface
- size_t solution_levels () const

    return size of subModel::solnControlCostMap
- void solution_level_cost_index (size_t cost_index)

    activate entry in subModel::solnControlCostMap
- size_t solution_level_cost_index () const

    return active entry in subModel::solnControlCostMap
- RealVector solution_level_costs () const

    return cost estimates from subModel::solnControlCostMap
- Real solution_level_cost () const

    return active cost estimate from subModel::solnControlCostMap
- void primary_response_fn_weights (const RealVector &wts, bool recurse_flag=true)

    set the relative weightings for multiple objective functions or least squares terms and optionally recurses into subModel
- void surrogate_function_indices (const SizetSet &surr_fn_indices)

    update the subModel's surrogate response function indices (DataFitSurrModel::surrogateFnIndices)
- void surrogate_response_mode (short mode)

    update the subModel's surrogate response mode (SurrogateModel::responseMode)
- short correction_type ()

retrieve subModel's correction type
- void correction_type (short corr_type)

  update subModel's correction type
- short correction_order ()

  retrieve subModel's correction order
- const RealVector & error_estimates ()

  retrieve error estimates corresponding to the subModel
- void build_approximation ()

  builds the subModel approximation
- bool build_approximation (const Variables &vars, const IntResponsePair &response_pr)

  builds the subModel approximation
- void rebuild_approximation ()

  updates a subModel approximation
- void update_approximation (bool rebuild_flag)

  replaces data in the subModel approximation
- void update_approximation (const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)

  replaces data in the subModel approximation
- void update_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)

  replaces data in the subModel approximation
- void append_approximation (bool rebuild_flag)

  appends data to the subModel approximation
- void append_approximation (const Variables &vars, const IntResponsePair &response_pr, bool rebuild_flag)

  appends data to the subModel approximation
- void append_approximation (const VariablesArray &vars_array, const IntResponseMap &resp_map, bool rebuild_flag)

  appends data to the subModel approximation
- void pop_approximation (bool save_surr_data, bool rebuild_flag=false)

  remove the previous data set addition to a surrogate (e.g., due to a previous append_approximation() call); flag manages storing of surrogate data for use in a subsequent push_approximation()
- void push_approximation ()

  push a previous approximation data state; reverse of pop_approximation
- bool push_available ()

  query for whether a trial increment is restorable within a surrogate
- void finalize_approximation ()

  finalize an approximation by applying all previous trial increments
- void combine_approximation ()

  combine the current approximation with previously stored data sets
- void combined_to_active (bool clear_combined=true)

  promote the combined approximation into the active approximation
- void clear_inactive ()

  clear inactive approximations (finalization + combination completed)
- std::vector< Approximation > & approximations ()

  retrieve the set of Approximations from the subModel
- const RealVectorArray & approximation_coefficients (bool normalized=false)

  retrieve the approximation coefficients from the subModel
- void approximation_coefficients (const RealVectorArray &approx_coeffs, bool normalized=false)

  set the approximation coefficients within the subModel
- const RealVector & approximation_variances (const Variables &vars)

  retrieve the approximation variances from the subModel
- const Pecos::SurrogateData & approximation_data (size_t fn_index)

retrieve the approximation data from the subModel

- void component_parallel_mode (short mode)

  RecastModel only supports parallelism in subModel, so this virtual function redefinition is simply a sanity check.
- size_t mi_parallel_level_index () const

  return subModel's MI parallel level index
- short local_eval_synchronization ()

  return subModel local synchronization setting
- int local_eval_concurrency ()

  return subModel local evaluation concurrency
- bool derived_master_overload () const

  flag which prevents overloading the master with a multiprocessor evaluation (request forwarded to subModel)
- IntIntPair estimate_partition_bounds (int max_eval_concurrency)

  estimate the minimum and maximum partition sizes that can be utilized by this Model
- void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set up RecastModel for parallel operations (request forwarded to subModel)
- void derived_init_serial ()

  set up RecastModel for serial operations (request forwarded to subModel).
- void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set active parallel configuration within subModel
- void derived_free_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  deallocate communicator partitions for the RecastModel (request forwarded to subModel)
- void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)

  Service subModel job requests received from the master. Completes when a termination message is received from stop_servers().
- void stop_servers ()

  executed by the master to terminate subModel server operations when RecastModel iteration is complete.
- void inactive_view (short view, bool recurse_flag=true)

  update the Model's inactive view based on higher level (nested) context and optionally recurse into subModel
- const String & interface_id () const

  return the subModel interface identifier
- bool evaluation_cache (bool recurse_flag=true) const

  if recurse_flag, return the subModel evaluation cache usage
- bool restart_file (bool recurse_flag=true) const

  if recurse_flag, return the subModel restart file usage
- int derived_evaluation_id () const

  return the current evaluation id for the RecastModel
- void set_evaluation_reference ()

  set the evaluation counter reference points for the RecastModel (request forwarded to subModel)
- void fine_grained_evaluation_counters ()

  request fine-grained evaluation reporting within subModel
- void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const

  print the evaluation summary for the RecastModel (request forwarded to subModel)
- void warm_start_flag (const bool flag)

  set the warm start flag, including the orderedModels
- void eval_tag_prefix (const String &eval_id_str)

  set the hierarchical eval ID tag prefix
- bool db_lookup (const Variables &search_vars, const ActiveSet &search_set, Response &found_resp)

  RecastModel may need to map variables, asv before DB lookup, or responses after lookup.
- virtual void assign_instance ()

  assign static pointer instance to this for use in static transformation functions

- virtual void init_metadata ()

    default clear metadata in Recasts; derived classes can override to no-op

- bool init_variables (const SizetArray &vars_comps_totals, const BitArray &all_relax_di, const BitArray &all_-relax_dr)

    initialize currentVariables and related info from the passed size/type info

- void init_response (size_t num_recast_primary_fns, size_t num_recast_secondary_fns, short recast_resp_-order, bool reshape_vars)

    initialize currentResponse from the passed size info

- void reshape_response (size_t num_recast_primary_fns, size_t num_recast_secondary_fns)

    Reshape the RecastModel Response, assuming no change in variables or derivative information.

- void init_constraints (size_t num_recast_secondary_fns, size_t recast_secondary_offset, bool reshape_vars)

    initialize userDefinedConstraints from the passed size info

- void update_from_model (Model &model)

    update current variables/bounds/labels/constraints from subModel

- virtual bool update_variables_from_model (Model &model)

    update active variables/bounds/labels from subModel

- void update_variable_values (const Model &model)

    update all variable values from passed sub-model

- void update_discrete_variable_values (const Model &model)

    update discrete variable values from passed sub-model

- void update_variable_bounds (const Model &model)

    update all variable bounds from passed sub-model

- void update_discrete_variable_bounds (const Model &model)

    update discrete variable bounds from passed sub-model

- void update_variable_labels (const Model &model)

    update all variable labels from passed sub-model

- void update_discrete_variable_labels (const Model &model)

    update discrete variable labels from passed sub-model

- void update_linear_constraints (const Model &model)

    update linear constraints from passed sub-model

- void update_variables_active_complement_from_model (Model &model)

    update complement of active variables/bounds/labels from subModel

- void update_response_from_model (Model &model)

    update labels and nonlinear constraint bounds/targets from subModel

- void update_secondary_response (const Model &model)

    update just secondary response from subModel

Static Protected Member Functions

- static short response_order (const Model &sub_model)

    helper to compute the recast response order during member initialization

- static String recast_model_id (const String &root_id, const String &type)

    Generate a model id for recast models.

Protected Attributes

- Model subModel

  the sub-model underlying the transformations
- int recastModelEvalCntr

  local evaluation id counter used for id mapping
- IntActiveSetMap recastSetMap

  map of recast active set passed to derived_evaluate_nowait(). Needed for currentResponse update in synchronization routines.
- IntVariablesMap recastVarsMap

  map of recast variables used by derived_evaluate_nowait(). Needed for primaryRespMapping() and secondaryRespMapping() in synchronization routines.
- IntVariablesMap subModelVarsMap

  map of subModel variables used by derived_evaluate_nowait(). Needed for primaryRespMapping() and secondaryRespMapping() in synchronization routines.
- IntResponseMap recastResponseMap

  map of recast responses used by RecastModel::derived_synchronize() and RecastModel::derived_synchronize_nowait()
- IntIntMap recastIdMap

  mapping from subModel evaluation ids to RecastModel evaluation ids
- bool nonlinearVarsMapping

  boolean set to true if the variables mapping involves a nonlinear transformation. Used in transform_set() to manage the requirement for gradients within the Hessian transformations. This does not require a BoolDeque for each individual variable, since response gradients and Hessians are managed per function, not per variable.

Static Protected Attributes

- static StringStringPairIntMap recastModelIdCounters

  Counters for naming RecastModels.

Private Member Functions

- void initialize_data_from_submodel ()

  code shared among constructors to initialize base class data from submodel
- void resize_response_mapping ()

  resize {primary,secondary}MapIndices and nonlinearRespMapping to synchronize with subModel sizes

Private Attributes

- Sizet2DArray varsMapIndices

  For each subModel variable, identifies the indices of the recast variables used to define it (maps RecastModel variables to subModel variables; data is packed with only the variable indices employed rather than a sparsely filled N_sm x N_r matrix).
- Sizet2DArray primaryRespMapIndices

  For each recast primary function, identifies the indices of the subModel functions used to define it (maps subModel response to RecastModel Response).
- Sizet2DArray secondaryRespMapIndices

  For each recast secondary function, identifies the indices of the subModel functions used to define it (maps subModel response to RecastModel response).
- BoolDequeArray nonlinearRespMapping

  array of BoolDeques, one for each recast response function. Each BoolDeque defines which subModel response functions contribute to the recast function using a nonlinear mapping. Used in transform_set() to augment the subModel function value/gradient requirements.

- RealVector mappedErrorEstimates

    mapping of subModel.error_estimates() through response mappings

- void(∗ variablesMapping)(const Variables &recast_vars, Variables &sub_model_vars)

    holds pointer for variables mapping function passed in ctor/initialize

- void(∗ setMapping)(const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)

    holds pointer for set mapping function passed in ctor/initialize

- void(∗ primaryRespMapping)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

    holds pointer for primary response mapping function passed in ctor/initialize

- void(∗ secondaryRespMapping)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response)

    holds pointer for secondary response mapping function passed in ctor/initialize

- void(∗ invVarsMapping)(const Variables &sub_model_vars, Variables &recast_vars)

    holds pointer for optional inverse variables mapping function passed in inverse_mappings()

- void(∗ invSetMapping)(const Variables &sub_model_vars, const ActiveSet &sub_model_set, ActiveSet &recast_set)

    holds pointer for optional inverse set mapping function passed in inverse_mappings()

- void(∗ invPriRespMapping)(const Variables &recast_vars, const Variables &sub_model_vars, const Response &recast_resp, Response &sub_model_resp)

    holds pointer for optional inverse primary response mapping function passed in inverse_mappings()

- void(∗ invSecRespMapping)(const Variables &recast_vars, const Variables &sub_model_vars, const Response &recast_resp, Response &sub_model_resp)

    holds pointer for optional inverse secondary response mapping function passed in inverse_mappings()

Additional Inherited Members

14.223.1 Detailed Description

Derived model class which provides a thin wrapper around a sub-model in order to recast the form of its inputs and/or outputs.

The RecastModel class uses function pointers to allow recasting of the subModel input/output into new problem forms. For example, this is used to recast SBO approximate subproblems, multiobjective and least-squares reductions, and variable/response.

For now, making the assumption that variables mappings are ordered by submodel active continous, discrete int, discrete string, discrete real variables, even though all current use cases are continuous only.

When not using the standard (full) constructor, client code must make sure to complete initialization before using the RecastModel's mapping functions. Initialization steps:

1. sub model (all ctors do this)
2. init_sizes: once known, size Variables, Response, Constraints (full and intermediate ctor do this)
3. init_maps: set indices and callback pointers (only full ctor does this)

14.223.2 Constructor & Destructor Documentation

14.223.2.1 RecastModel (const Model & *sub_model,* const Sizet2DArray & *vars_map_indices,* const SizetArray & *vars_comps_totals,* const BitArray & *all_relax_di,* const BitArray & *all_relax_dr,* bool *nonlinear_vars_mapping,* void(∗)(const Variables &recast_vars, Variables &sub_model_vars) *variables_map,* void(∗)(const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set) *set_map,* const Sizet2DArray & *primary_resp_map_indices,* const Sizet2DArray & *secondary_resp_map_indices,* size_t *recast_secondary_offset,* short *recast_resp_order,* const BoolDequeArray & *nonlinear_resp_mapping,* void(∗)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response) *primary_resp_map,* void(∗)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response) *secondary_resp_map*)

standard (full) constructor; assumes provided sizes and map functions are final and constructs all member data

Default recast model constructor. Requires full definition of the transformation; if any mappings are NULL, they are assumed to remain so in later initialization or updates. Parameter vars_comps_totals indicates the number of each type of variable {4 types} x {3 domains} in the recast variable space. Note: recast_secondary_offset is the start index for equality constraints, typically num nonlinear ineq constraints.

References Dakota::abort_handler(), Response::copy(), Variables::copy(), Model::current_response(), Model::current_variables(), Model::currentResponse, Model::currentVariables, Variables::cv(), RecastModel::init_constraints(), RecastModel::init_metadata(), RecastModel::init_response(), RecastModel::init_variables(), RecastModel::initialize_data_from_submodel(), Model::modelId, Model::modelType, RecastModel::nonlinearRespMapping, Response::num_functions(), Model::numDerivVars, Model::numFns, RecastModel::primaryRespMapIndices, RecastModel::primaryRespMapping, RecastModel::recast_model_id(), RecastModel::root_model_id(), RecastModel::secondaryRespMapIndices, RecastModel::secondaryRespMapping, RecastModel::subModel, Model::supportsEstimDerivs, and RecastModel::variablesMapping.

14.223.2.2 RecastModel (const Model & *sub_model,* const SizetArray & *vars_comps_totals,* const BitArray & *all_relax_di,* const BitArray & *all_relax_dr,* size_t *num_recast_primary_fns,* size_t *num_recast_secondary_fns,* size_t *recast_secondary_offset,* short *recast_resp_order*)

alternate constructor; uses provided sizes to construct Variables, Response and Constraints so Model can be passed to an Iterator; requires subsequent init_maps() call.

This alternate constructor defers initialization of the function pointers until a separate call to initialize(), and accepts the minimum information needed to construct currentVariables, currentResponse, and userDefinedConstraints. The resulting model is sufficiently complete for passing to an Iterator. Parameter vars_comps_totals indicates the number of each type of variable {4 types} x {3 domains} in the recast variable space. Note: recast_secondary_offset is the start index for equality constraints, typically num nonlinear ineq constraints.

References RecastModel::init_sizes(), RecastModel::initialize_data_from_submodel(), Model::modelId, Model::modelType, RecastModel::recast_model_id(), RecastModel::root_model_id(), and Model::supportsEstimDerivs.

14.223.3 Member Function Documentation

14.223.3.1 void init_maps (const Sizet2DArray & *vars_map_indices,* bool *nonlinear_vars_mapping,* void(∗)(const Variables &recast_vars, Variables &sub_model_vars) *variables_map,* void(∗)(const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set) *set_map,* const Sizet2DArray & *primary_resp_map_indices,* const Sizet2DArray & *secondary_resp_map_indices,* const BoolDequeArray & *nonlinear_resp_mapping,* void(∗)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response) *primary_resp_map,* void(∗)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response) *secondary_resp_map*)

initialize recast indices and map callbacks after alternate construction

This function is used for late initialization of the recasting functions. It is used in concert with the alternate constructor.

References Dakota::abort_handler(), RecastModel::nonlinearRespMapping, RecastModel::nonlinearVarsMapping, RecastModel::primaryRespMapIndices, RecastModel::primaryRespMapping, RecastModel::secondaryRespMap-

Indices, RecastModel::secondaryRespMapping, RecastModel::setMapping, RecastModel::variablesMapping, and RecastModel::varsMapIndices.

Referenced by EffGlobalMinimizer::construct_batch_acquisition(), EffGlobalMinimizer::construct_batch_exploration(), DataTransformModel::DataTransformModel(), SubspaceModel::initialize_base_recast(), RandomFieldModel::initialize_recast(), ProbabilityTransformModel::ProbabilityTransformModel(), ScalingModel::ScalingModel(), and WeightingModel::WeightingModel().

14.223.3.2 void derived_evaluate (const ActiveSet & *set*) [protected], [virtual]

portion of evaluate() specific to RecastModel (forward to subModel.evaluate())

The RecastModel is evaluated by an Iterator for a recast problem formulation. Therefore, the currentVariables, incoming active set, and output currentResponse all correspond to the recast inputs/outputs.

Reimplemented from Model.

Reimplemented in SubspaceModel.

References Response::active_set(), Model::current_response(), Model::current_variables(), Model::currentResponse, Model::currentVariables, Model::evaluate(), RecastModel::primaryRespMapping, RecastModel::recastModelEvalCntr, RecastModel::secondaryRespMapping, RecastModel::subModel, RecastModel::transform_response(), RecastModel::transform_set(), RecastModel::transform_variables(), and Response::update().

Referenced by SubspaceModel::derived_evaluate(), ActiveSubspaceModel::derived_evaluate(), DataTransformModel::derived_evaluate(), and RandomFieldModel::derived_evaluate().

14.223.3.3 void eval_tag_prefix (const String & *eval_id_str*) [inline], [protected], [virtual]

set the hierarchical eval ID tag prefix

RecastModel just forwards any tags to its subModel

Reimplemented from Model.

References Model::eval_tag_prefix(), and RecastModel::subModel.

14.223.3.4 void update_from_model (Model & *model*) [protected]

update current variables/bounds/labels/constraints from subModel

Update inactive values and labels in currentVariables and inactive bound constraints in userDefinedConstraints from variables and constraints data within subModel.

References RecastModel::update_response_from_model(), RecastModel::update_variables_active_complement_from_model(), and RecastModel::update_variables_from_model().

Referenced by ProbabilityTransformModel::update_from_subordinate_model(), and RecastModel::update_from_subordinate_model().

The documentation for this class was generated from the following files:

- RecastModel.hpp
- RecastModel.cpp

14.224 ReducedBasis Class Reference

Public Member Functions

- ReducedBasis ()

  default constructor

- void **set_matrix** (const RealMatrix &)
- const RealMatrix & **get_matrix** ()
- void center_matrix ()

  center the matrix by scaling each column by its means
- void update_svd (bool center_matrix_by_col_means=true)

  ensure that the factorization is current, centering if requested
- bool **is_valid** () const
- const Real & **get_singular_values_sum** () const
- const Real & **get_eigen_values_sum** () const
- const RealVector & **get_column_means** ()
- const RealVector & **get_singular_values** () const
- RealVector **get_singular_values** (const TruncationCondition &) const
- const RealMatrix & get_left_singular_vector () const

  the num_observations n x num_observations n orthogonal matrix U; the left singular vectors are the first min(n,p) columns
- const RealMatrix & get_right_singular_vector_transpose () const

  the num_responses p x num_responses p orthogonal matrix V'; the right singular vectors are the first min(n,p) rows of V' (columns of V)

Private Attributes

- RealMatrix **matrix**
- RealMatrix **workingMatrix**
- RealMatrix **U_matrix**
- RealVector **S_values**
- RealMatrix **VT_matrix**
- RealVector **column_means**
- bool **col_means_computed**
- bool **is_centered**
- bool **is_valid_svd**
- Real **singular_values_sum**
- Real **eigen_values_sum**
- TruncationCondition ∗ **truncation**

14.224.1 Detailed Description

The ReducedBasis class is used to ... (TODO - RWH)

Class to manage data-driven dimension reduction. The passed matrix with num_observations n rows and num_-responses p columns contains realizations of a set of responses. The class optionally centers the matrix by the column means. Stores a singular value decomposition of the passsed data matrix X = U∗S∗V', which can also be used for PCA, where we seek an eigendecomposition of the covariance: X'∗X = V∗D∗V^{-1} = V∗S^2∗V'

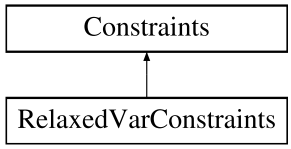
The documentation for this class was generated from the following files:

- ReducedBasis.hpp
- ReducedBasis.cpp

14.225 RelaxedVarConstraints Class Reference

Derived class within the Constraints hierarchy which employs relaxation of discrete variables.

Inheritance diagram for RelaxedVarConstraints:



Public Member Functions

- RelaxedVarConstraints (const SharedVariablesData &svd)
  lightweight constructor
- RelaxedVarConstraints (const ProblemDescDB &problem_db, const SharedVariablesData &svd)
  standard constructor
- ∼RelaxedVarConstraints ()
  destructor
- void write (std::ostream &s) const
  write a variable constraints object to an std::ostream
- void read (std::istream &s)
  read a variable constraints object from an std::istream

Additional Inherited Members

14.225.1 Detailed Description

Derived class within the Constraints hierarchy which employs relaxation of discrete variables.

Derived variable constraints classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The RelaxedVarConstraints derived class combines continuous and discrete domain types through integer relaxation. The branch and bound method uses this approach (see Variables::get_-variables(problem_db) for variables type selection; variables type is passed to the Constraints constructor in Model).

14.225.2 Constructor & Destructor Documentation

14.225.2.1 RelaxedVarConstraints (const ProblemDescDB & *problem_db,* const SharedVariablesData & *svd*)

standard constructor

In this class, a relaxed data approach is used in which continuous and discrete arrays are combined into a single continuous array (integrality is relaxed; the converse of truncating reals is not currently supported but could be in the future if needed). Iterators which use this class include: BranchBndOptimizer.

References SharedVariablesData::all_relaxed_discrete_int(), SharedVariablesData::all_relaxed_discrete_real(), Constraints::allContinuousLowerBnds, Constraints::allContinuousUpperBnds, Constraints::allDiscreteIntLower-Bnds, Constraints::allDiscreteIntUpperBnds, Constraints::allDiscreteRealLowerBnds, Constraints::allDiscreteReal-UpperBnds, Dakota::copy_data_partial(), ProblemDescDB::get_iv(), ProblemDescDB::get_rv(), and Constraints-::sharedVarsData.

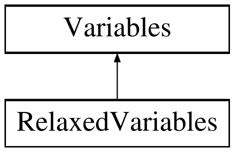
The documentation for this class was generated from the following files:

- RelaxedVarConstraints.hpp
- RelaxedVarConstraints.cpp

14.226 RelaxedVariables Class Reference

Derived class within the Variables hierarchy which employs the relaxation of discrete variables.

Inheritance diagram for RelaxedVariables:



Public Member Functions

- RelaxedVariables (const ProblemDescDB &problem_db, const std::pair< short, short > &view)

  standard constructor
- RelaxedVariables (const SharedVariablesData &svd)

  lightweight constructor
- ∼RelaxedVariables ()

  destructor

Protected Member Functions

- void read (std::istream &s)

  read a variables object from an std::istream
- void read_tabular (std::istream &s, unsigned short vars_part=ALL_VARS)
- void write (std::ostream &s, unsigned short vars_part=ALL_VARS) const

  write a variables object to an std::ostream, e.g., the console, optionally specifying which partition (all/active/inactive)
- void write_aprepro (std::ostream &s) const

  write a variables object to an std::ostream in aprepro format, e.g., a parameters file
- void write_tabular (std::ostream &s, unsigned short vars_part=ALL_VARS) const

  write a variables object in tabular format to an std::ostream, optionally specifying which partition (all/active/inactive)
- void write_tabular_partial (std::ostream &s, size_t start_index, size_t num_items) const

  write range of variables in tabular format to an std::ostream
- void write_tabular_labels (std::ostream &s, unsigned short vars_part=ALL_VARS) const

  write the labels in input spec order to a std::ostream, optionally specifying which partition (all/active/inactive)
- void write_tabular_partial_labels (std::ostream &s, size_t start_index, size_t num_items) const

  write range of variable labels in input spec order to a std::ostream
- template<typename Reader >
  void read_core (std::istream &s, Reader read_handler, unsigned short vars_part)

  Implementation of reading various formats using the specified read handler, accounting for reordering due to relaxation.
- template<typename Writer >
  void write_core (std::ostream &s, Writer write_handler, unsigned short vars_part) const

  Implementation of writing various formats using the specified write handler, accounting for reordering due to relaxation.
- template<typename Writer >
  bool write_partial_core (std::ostream &s, Writer write_handler, size_t start_index, size_t end_index, size_t &acv_offset, size_t &adiv_offset, size_t &adsv_offset, size_t &adrv_offset, size_t &av_cntr, size_t num_cv, size_t num_div, size_t num_dsv, size_t num_drv) const

  Implementation for partial writing in various formats using the specified write handler.

Additional Inherited Members

14.226.1 Detailed Description

Derived class within the Variables hierarchy which employs the relaxation of discrete variables.

Derived variables classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The RelaxedVariables derived class combines continuous and discrete domain types but separates design, uncertain, and state variable types. The branch and bound method uses this approach (see Variables::get_variables(problem_db)).

14.226.2 Constructor & Destructor Documentation

14.226.2.1 RelaxedVariables (const ProblemDescDB & *problem_db*, const std::pair< short, short > & *view*)

standard constructor

In this class, a relaxed data approach is used in which continuous and discrete arrays are combined into a single continuous array (integrality is relaxed; the converse of truncating reals is not currently supported but could be in the future if needed). Iterators/strategies which use this class include: BranchBndOptimizer. Extract fundamental variable types and labels and merge continuous and discrete domains to create aggregate arrays and views.

References SharedVariablesData::all_relaxed_discrete_int(), SharedVariablesData::all_relaxed_discrete_real(), Variables::allContinuousVars, Variables::allDiscreteIntVars, Variables::allDiscreteRealVars, Variables::allDiscreteStringVars, Dakota::copy_data_partial(), ProblemDescDB::get_iv(), ProblemDescDB::get_rv(), ProblemDescDB::get_sa(), and Variables::sharedVarsData.

14.226.3 Member Function Documentation

14.226.3.1 void read_tabular (std::istream & *s*, unsigned short *vars_part* = ALL_VARS) [protected], [virtual]

Presumes variables object is appropriately sized to receive data

Reimplemented from Variables.

References RelaxedVariables::read_core().

14.226.3.2 void read_core (std::istream & *s*, Reader *read_handler*, unsigned short *vars_part*) [protected]

Implementation of reading various formats using the specified read handler, accounting for reordering due to relaxation.

Reordering is required in all read/write cases that will be visible to the user since all derived vars classes should use the same ordering for clarity. Neutral file I/O, binary streams, and packed buffers do not need to reorder (so long as read/write are consistent) since this data is not intended for public consumption.

References SharedVariablesData::active_components_totals(), Variables::all_continuous_variable_labels(), Variables::all_discrete_int_variable_labels(), Variables::all_discrete_real_variable_labels(), Variables::all_discrete_string_variable_labels(), SharedVariablesData::all_relaxed_discrete_int(), SharedVariablesData::all_relaxed_discrete_real(), Variables::allContinuousVars, Variables::allDiscreteIntVars, Variables::allDiscreteRealVars, Variables::allDiscreteStringVars, SharedVariablesData::components_totals(), SharedVariablesData::cv_start(), SharedVariablesData::div_start(), SharedVariablesData::drv_start(), SharedVariablesData::dsv_start(), SharedVariablesData::icv_start(), SharedVariablesData::idiv_start(), SharedVariablesData::idrv_start(), SharedVariablesData::idsv_start(), SharedVariablesData::inactive_components_totals(), and Variables::sharedVarsData.

Referenced by RelaxedVariables::read(), and RelaxedVariables::read_tabular().

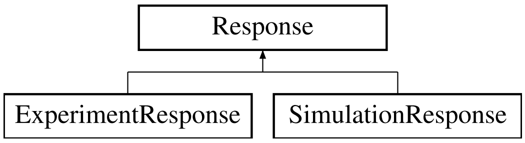
The documentation for this class was generated from the following files:

- RelaxedVariables.hpp
- RelaxedVariables.cpp

14.227 Response Class Reference

Container class for response functions and their derivatives. Response provides the enveloper base class.

Inheritance diagram for Response:



Public Member Functions

- Response ()
  default constructor
- Response (short type, const Variables &vars, const ProblemDescDB &problem_db)
  standard constructor built from problem description database
- Response (const SharedResponseData &srd, const ActiveSet &set)
  alternate constructor that shares response data
- Response (short type, const ActiveSet &set)
  alternate constructor using limited data without sharing
- Response (const SharedResponseData &srd)
  alternate constructor using limited data (explicit disallows implicit type conversion)
- Response (const Response &response)
  copy constructor
- virtual ∼Response ()
  destructor
- Response operator= (const Response &response)
  assignment operator
- const SharedResponseData & shared_data () const
  return sharedRespData
- SharedResponseData & shared_data ()
  return sharedRespData
- size_t num_functions () const
  return the number of response functions
- const ActiveSet & active_set () const
  return the active set
- void active_set (const ActiveSet &set)
  set the active set
- const ShortArray & active_set_request_vector () const
  return the active set request vector
- ShortArray & active_set_request_vector ()
  return the active set request vector
- void active_set_request_vector (const ShortArray &asrv)
  set the active set request vector and verify consistent number of response functions
- const SizetArray & active_set_derivative_vector () const

return the active set derivative vector

- SizetArray & active_set_derivative_vector ()

  return the active set derivative vector
- void active_set_derivative_vector (const SizetArray &asdv)

  set the active set derivative vector and reshape functionGradients/functionHessians if needed
- const Real & function_value (size_t i) const

  return a function value
- Real & function_value_view (size_t i)

  return a "view" of a function value for updating in place
- const RealVector & function_values () const

  return all function values
- RealVector function_values_view ()

  return all function values as a view for updating in place
- RealVector function_values_view () const

  return all function values as a view for accessing the function values vector from a const response
- void function_value (const Real &fn_val, size_t i)

  set a function value
- void function_values (const RealVector &fn_vals)

  set all function values
- const Real ∗ function_gradient (int i) const

  return the i-th function gradient as a const Real∗
- RealVector function_gradient_view (int i)

  return the i-th function gradient as a SerialDenseVector view (shallow copy) for updating in place
- RealVector function_gradient_view (int i) const

  return the i-th function gradient as a SerialDenseVector view (shallow copy) for accessing a column vector from a const matrix
- RealVector function_gradient_copy (int i) const

  return the i-th function gradient as a SerialDenseVector Teuchos::Copy (deep copy)
- const RealMatrix & function_gradients () const

  return all function gradients
- RealMatrix function_gradients_view ()

  return all function gradients as a view for updating in place
- RealMatrix function_gradients_view () const

  return all function gradients as a view for updating in place
- void function_gradient (const RealVector &fn_grad, int i)

  set a function gradient
- void function_gradients (const RealMatrix &fn_grads)

  set all function gradients
- const RealSymMatrix & function_hessian (size_t i) const

  return the i-th function Hessian
- RealSymMatrix function_hessian_view (size_t i)

  return the i-th function Hessian as a Teuchos::View (shallow copy) for updating in place
- RealSymMatrix function_hessian_view (size_t i) const

  return the i-th function Hessian as a Teuchos::View (shallow copy) for accessing the i-th matrix within a const matrix array
- const RealSymMatrixArray & function_hessians () const

  return all function Hessians
- RealSymMatrixArray function_hessians_view ()

  return all function Hessians as Teuchos::Views (shallow copies) for updating in place
- RealSymMatrixArray function_hessians_view () const

  return all function Hessians as Teuchos::Views (shallow copies) for updating in place

- void function_hessian (const RealSymMatrix &fn_hessian, size_t i)

  set a function Hessian
- void function_hessians (const RealSymMatrixArray &fn_hessians)

  set all function Hessians
- const IntVector & field_lengths () const

  return the field lengths (from SharedResponseData)
- void field_lengths (const IntVector &field_lens)

  set the field lengths (within SharedResponseData)
- RealVector field_values_view (size_t i) const

  return const field values for the i-th field
- RealVector field_values_view (size_t i)

  return a "view" of the i-th field values for updating in place
- void field_values (const RealVector &field_val, size_t i)

  set the values for the i-th field
- RealMatrix field_gradients_view (size_t i) const

  return a view of the gradients of each element of the i-th field
- RealSymMatrixArray field_hessians_view (size_t i) const

  return a view of the hessians of each element of the i-th field
- RealMatrix field_coords_view (size_t i)

  return a "view" of the i-th field's coordinates
- const RealMatrix field_coords_view (size_t i) const

  return a const "view" of the i-th field's coordinates
- void field_coords (const RealMatrix &field_coords, size_t i)

  set the i-th field's coordinates
- const IntVector & num_coords_per_field () const

  return the number of coordinates each field has (from SharedResponseData)
- const StringArray & function_labels () const

  return the fine-grained (unrolled) response function identifier strings from sharedRespData
- void function_labels (const StringArray &labels)

  set the fine-grained (unrolled) response function identifier strings within sharedRespData
- const StringArray & field_group_labels ()

  return the user-provided field group labels instead of the unrolled labels available through function_labels()
- const std::vector
  < RespMetadataT > & metadata () const

  get the (possibly empty) response metadata; (get labels through shared_data())
- void metadata (const std::vector< RespMetadataT > &md)

  set the response metadata (set labels through shared_data())
- void metadata (const std::vector< RespMetadataT > &md, size_t start)

  set a portion of the response metadata starting from given position
- void read (std::istream &s, const unsigned short format=FLEXIBLE_RESULTS)

  read a response object of specified format from a std::istream
- void write (std::ostream &s) const

  write a response object to a std::ostream
- void read_annotated (std::istream &s)

  read a response object in annotated format from a std::istream
- void write_annotated (std::ostream &s) const

  write a response object in annotated format to a std::ostream
- void read_tabular (std::istream &s)

  read responseRep::functionValues in tabular format from a std::istream
- void write_tabular (std::ostream &s, bool eol=true) const

  write responseRep::functionValues in tabular format to a std::ostream

- void write_tabular_partial (std::ostream &s, size_t start_index, size_t num_items) const

  write portion of responseRep::functionValues in tabular format to a std::ostream
- void write_tabular_labels (std::ostream &s, bool eol=true) const

  write the response labels in tabular format to a std::ostream
- void read (MPIUnpackBuffer &s)

  read a response object from a packed MPI buffer
- void write (MPIPackBuffer &s) const

  write a response object to a packed MPI buffer
- Response copy (bool deep_srd=false) const

  return a deep response copy of the contained responseRep for use in history mechanisms (SharedResponseData uses a shallow copy by default)
- int data_size ()

  return the number of doubles active in response. Used for sizing double∗ response_data arrays passed into read_data and write_data.
- void read_data (double ∗response_data)

  read from an incoming double∗ array
- void write_data (double ∗response_data)

  write to an incoming double∗ array
- void overlay (const Response &response)

  add incoming response to functionValues/Gradients/Hessians
- void update (const Response &response, bool pull_metadata=false)

  Used in place of operator= when only results data updates are desired (functionValues/functionGradients/functionHessians are updated, ASV/labels/id's/etc. are not). Care is taken to allow different derivative array sizing between the two response objects.
- void update (const RealVector &source_fn_vals, const RealMatrix &source_fn_grads, const RealSymMatrixArray &source_fn_hessians, const ActiveSet &source_set)

  Overloaded form which allows update from components of a response object. Care is taken to allow different derivative array sizing.
- void update_partial (size_t start_index_target, size_t num_items, const Response &response, size_t start_index_source)

  partial update of this response object from another response object. The response objects may have different numbers of response functions.
- void update_partial (size_t start_index_target, size_t num_items, const RealVector &source_fn_vals, const RealMatrix &source_fn_grads, const RealSymMatrixArray &source_fn_hessians, const ActiveSet &source_set, size_t start_index_source)

  Overloaded form which allows partial update from components of a response object. The response objects may have different numbers of response functions.
- void reshape (size_t num_fns, size_t num_params, bool grad_flag, bool hess_flag)

  rehapes response data arrays
- void reshape_metadata (size_t num_meta)

  rehapes response metadata arrays
- void reset ()

  resets all response data to zero
- void reset_inactive ()

  resets all inactive response data to zero
- bool is_null () const

  function to check responseRep (does this handle contain a body)
- virtual void set_scalar_covariance (RealVector &scalars)

  method to set the covariance matrix defined for ExperimentResponse
- virtual const ExperimentCovariance & experiment_covariance () const

  retrieve the ExperimentCovariance structure

- virtual void set_full_covariance (std::vector< RealMatrix > &matrices, std::vector< RealVector > &diagonals, RealVector &scalars, IntVector matrix_map_indices, IntVector diagonal_map_indices, IntVector scalar_map_indices)

  method to set the full covariance matrices for ExperimentResponse
- virtual Real apply_covariance (const RealVector &residuals) const

  method to compute the triple product v'∗inv(C)∗v.
- virtual void apply_covariance_inv_sqrt (const RealVector &residuals, RealVector &weighted_residuals) const

  method to compute (v'∗inv(C)^1/2), to compute weighted residual
- virtual void **apply_covariance_inv_sqrt** (const RealMatrix &gradients, RealMatrix &weighted_gradients) const
- virtual void **apply_covariance_inv_sqrt** (const RealSymMatrixArray &hessians, RealSymMatrixArray &weighted_hessians) const
- virtual void **get_covariance_diagonal** (RealVector &diagonal) const
- virtual Real covariance_determinant () const

  covariance determinant for one experiment (default 1.0)
- virtual Real log_covariance_determinant () const

  log of covariance determinant for one experiment (default 0.0)

Protected Member Functions

- Response (BaseConstructor, const Variables &vars, const ProblemDescDB &problem_db)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- Response (BaseConstructor, const SharedResponseData &srd, const ActiveSet &set)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- Response (BaseConstructor, const ActiveSet &set)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- Response (BaseConstructor, const SharedResponseData &srd)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- virtual void copy_rep (std::shared_ptr< Response > source_resp_rep)

  Implementation of data copy for Response letters (specialized by some derived letter types); pulls base class data from source_resp_rep into the this object.

Protected Attributes

- SharedResponseData sharedRespData

  reference-counted instance of shared response data: id's, labels
- RealVector functionValues

  Abstract set of response functions. Ordered: [primary_scalar, primary_field, nonlinear_inequality, nonlinear_equality].
- RealMatrix functionGradients

  first derivatives of the response functions
- RealSymMatrixArray functionHessians

  second derivatives of the response functions
- IntRealMatrixMap fieldCoords

  coordinates (independent vars like x,t) on which field values depend
- ActiveSet responseActiveSet

  copy of the ActiveSet used by the Model to generate a Response instance
- std::vector< RespMetadataT > metaData

  metadata storage

Private Member Functions

- template<class Archive , typename OrdinalType , typename ScalarType >
  void write_sdm_col (Archive &ar, int col, const Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > &sdm) const

  write a column of a SerialDenseMatrix
- template<class Archive , typename OrdinalType , typename ScalarType >
  void read_sdm_col (Archive &ar, int col, Teuchos::SerialDenseMatrix< OrdinalType, ScalarType > &sdm)

  read a column of a SerialDenseMatrix
- template<class Archive >
  void load (Archive &ar, const unsigned int version)

  read a Response from an archive<class Archive>
- template<class Archive >
  void load_rep (Archive &ar, const unsigned int version)

  read a Response letter object from an archive
- template<class Archive >
  void save (Archive &ar, const unsigned int version) const

  write a Response to an archive
- template<class Archive >
  void save_rep (Archive &ar, const unsigned int version) const

  write a Response letter object to an archive
- BOOST_SERIALIZATION_SPLIT_MEMBER()
  std std::shared_ptr< Response > get_response (const SharedResponseData &srd, const ActiveSet &set) const

  Used by standard envelope constructor to instantiate a new letter class.
- std::shared_ptr< Response > get_response (short type, const ActiveSet &set) const

  Used by alternate envelope constructor to instantiate a new letter class.
- std::shared_ptr< Response > get_response (const SharedResponseData &srd) const

  Used by copy() to instantiate a new letter class.
- std::shared_ptr< Response > get_response (short type) const

  Used by read functions to instantiate a new letter class.
- void read_annotated_rep (std::istream &s)

  read a letter object in annotated format from a std::istream
- void write_annotated_rep (std::ostream &s) const

  write a letter object in annotated format to a std::ostream
- void read_rep (MPIUnpackBuffer &s)

  read a letter object from a packed MPI buffer
- void write_rep (MPIPackBuffer &s) const

  write a letter object to a packed MPI buffer
- void shape_rep (const ActiveSet &set, bool initialize=true)

  resizes the representation's containers
- void reshape_rep (size_t num_fns, size_t num_params, bool grad_flag, bool hess_flag)

  resizes the representation's containers
- void **read_core** (std::istream &s, const unsigned short formats, std::ostringstream &errors)
- bool **expect_derivatives** (const ShortArray &asv)
- void read_gradients (std::istream &s, const ShortArray &asv, bool expect_metadata, std::ostringstream &error)

  Read gradients from a freeform stream. Insert error messages.
- void read_hessians (std::istream &s, const ShortArray &asv, bool expect_metadata, std::ostringstream &error)

  Read Hessians from a freeform stream. Insert error messages.
- void read_labeled_fn_vals (std::istream &s, const ShortArray &asv, size_t num_metadata, std::ostringstream &errors)

Read function values from an annotated stream. Insert error messages.

- void read_flexible_fn_vals (std::istream &s, const ShortArray &asv, size_t num_metadata, std::ostringstream &errors)

  Read function values from a stream in a "flexible" way – ignoring any labels. Insert error messages into errors stream.

- bool failure_reported (std::istream &s)

  Check for FAIL in stream.

Private Attributes

- std::shared_ptr< Response > responseRep

  pointer to the body (handle-body idiom)

Friends

- class **boost::serialization::access**
- bool operator== (const Response &resp1, const Response &resp2)

  equality operator

- bool operator!= (const Response &resp1, const Response &resp2)

  inequality operator

14.227.1 Detailed Description

Container class for response functions and their derivatives. Response provides the enveloper base class.

The Response class is a container class for an abstract set of functions (functionValues) and their first (functionGradients) and second (functionHessians) derivatives. The functions may involve objective and constraint functions (optimization data set), least squares terms (parameter estimation data set), or generic response functions (uncertainty quantification data set). When field responses are present, the stored response elements are ordered: [primary_scalar, primary_field, nonlinear_inequality, nonlinear_equality].

For memory efficiency, it employs the "letter-envelope idiom" approach to reference counting and representation sharing (see Coplien "Advanced C++"), for which the base Response class serves as the envelope and one of its derived classes serves as the letter.

14.227.2 Member Function Documentation

14.227.2.1 BOOST_SERIALIZATION_SPLIT_MEMBER () std std::shared_ptr< Response > get_response (const SharedResponseData & *srd*, const ActiveSet & *set*) const [private]

Used by standard envelope constructor to instantiate a new letter class.

Used by alternate envelope constructor to instantiate a new letter class

14.227.3 Member Data Documentation

14.227.3.1 RealMatrix functionGradients [protected]

first derivatives of the response functions

the gradient vectors (plural) are column vectors in the matrix (singular) with (row, col) = (variable index, response fn index).

Referenced by Response::field_gradients_view(), Response::function_gradient(), Response::function_gradient_copy(), Response::function_gradient_view(), Response::function_gradients(), and Response::function_gradients_view().

The documentation for this class was generated from the following file:

- DakotaResponse.hpp

14.228 RestartWriter Class Reference

Public Member Functions

- RestartWriter ()

    optional default ctor allowing a non-outputting RestartWriter
- RestartWriter (const String &write_restart_filename)

    typical ctor taking a filename; this class encapsulates the output stream
- RestartWriter (std::ostream &write_restart_stream)

    alternate ctor taking a stream, helpful for testing; assumes client manages the output stream
- const String & filename ()

    output filename for this writer
- void append_prp (const ParamResponsePair &prp_in)

    add the passed pair to the restart file
- void flush ()

    flush the restart stream so we have a complete restart record should Dakota abort

Private Member Functions

- RestartWriter (const RestartWriter &)

    copy constructor is disallowed due to file stream
- const RestartWriter & operator= (const RestartWriter &)

    assignment is disallowed due to file stream

Private Attributes

- String restartOutputFilename

    the name of the restart output file
- std::ofstream restartOutputFS

    Binary stream to which restart data is written.
- std::unique_ptr
  $<$ boost::archive::binary_oarchive $>$ restartOutputArchive

    Binary output archive to which data is written (pointer since no default ctor for oarchive and may not be initialized);.

14.228.1 Detailed Description

Component for writing restart files. Creation and destruction of archive and associated stream are managed here.

The documentation for this class was generated from the following files:

- OutputManager.hpp
- OutputManager.cpp

14.229 ResultAttribute$<$ T $>$ Struct Template Reference

Data structure for a single Real, String, or int valued attribute.

Public Member Functions

- ResultAttribute (const String &label, const T &value)

  Construct an attribute.

Public Attributes

- String label

  Key for the attribute.
- T value

  Value for the attribute.

14.229.1 Detailed Description

template<typename T>struct Dakota::ResultAttribute< T >

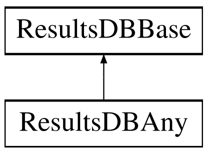
Data structure for a single Real, String, or int valued attribute.

The documentation for this struct was generated from the following file:

- dakota_results_types.hpp

14.230 ResultsDBAny Class Reference

Inheritance diagram for ResultsDBAny:



Public Member Functions

- **ResultsDBAny** (const String &filename)
- void insert (const StrStrSizet &iterator_id, const std::string &data_name, const boost::any &result, const MetaDataType &metadata) override

  record addition with metadata map
- void flush () const

  Write data to file.
- void insert (const StrStrSizet &iterator_id, const StringArray &location, const boost::any &data, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray(), const bool &transpose=false) override

  insert an arbitrary type (RealMatrix) with metadata
- void allocate_vector (const StrStrSizet &iterator_id, const StringArray &location, ResultsOutputType stored_type, const int &len, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray())

  Pre-allocate a vector and (optionally) attach dimension scales and attributes. Insert elements using insert_into(...)
- void allocate_matrix (const StrStrSizet &iterator_id, const StringArray &location, ResultsOutputType stored_type, const int &num_rows, const int &num_cols, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray())

Pre-allocate a matrix and (optionally) attach dimension scales and attributes. Insert rows or columns using insert_-into(...)

- void insert_into (const StrStrSizet &iterator_id, const StringArray &location, const boost::any &data, const int &index, const bool &row)

  Insert a row or column into a pre-allocated matrix.
- void add_metadata_to_method (const StrStrSizet &iterator_id, const AttributeArray &attrs) override

  Add key:value metadata to method.
- void add_metadata_to_execution (const StrStrSizet &iterator_id, const AttributeArray &attrs) override

  Add key:value metadata to execution.
- void add_metadata_to_object (const StrStrSizet &iterator_id, const StringArray &location, const Attribute-Array &attrs) override

  Associate key:value metadata with the object at the location.
- void add_metadata_to_study (const AttributeArray &attrs) override

  Associate key:value metadata with the study.

Private Member Functions

- void print_metadata (std::ostream &os, const MetaDataType &md) const

  print metadata to ostream
- void extract_data (const boost::any &dataholder, std::ostream &os) const

  determine the type of contained data and output it to ostream
- void output_data (const std::vector< double > &data, std::ostream &os) const

  output data to ostream
- void output_data (const std::vector< RealVector > &data, std::ostream &os) const

  output data to ostream
- void output_data (const std::vector< std::string > &data, std::ostream &os) const

  output data to ostream
- void output_data (const std::vector< std::vector< std::string > > &data, std::ostream &os) const

  output data to ostream
- void output_data (const std::vector< RealMatrix > &data, std::ostream &os) const

  output data to ostream
- void output_data (const RealMatrix &data, std::ostream &os) const

  output data to ostream

Private Attributes

- String fileName

  name of database file

Additional Inherited Members

14.230.1 Detailed Description

Class: ResultsDBAny

Description: A map-based container to store DAKOTA Iterator results in underlying boost::anys, with optional meta-data

14.230.2 Member Function Documentation

14.230.2.1 void insert (const StrStrSizet & *iterator_id,* const std::string & *data_name,* const boost::any & *result,* const MetaDataType & *metadata*) [override], [virtual]

record addition with metadata map

Add or update existing entry

Implements ResultsDBBase.

References ResultsDBBase::iteratorData, and Dakota::make_key().

14.230.2.2 void extract_data (const boost::any & *dataholder,* std::ostream & *os*) const [private]

determine the type of contained data and output it to ostream

Extract the data from the held any and map to supported concrete types int double RealVector (Teuchos::SerialDenseVector<int,double>) RealMatrix (Teuchos::SerialDenseMatrix<int,double>)

References ResultsDBAny::output_data().

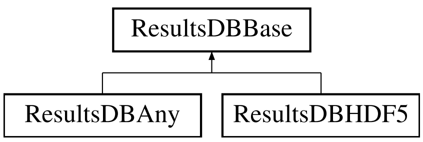
Referenced by ResultsDBAny::flush().

The documentation for this class was generated from the following files:

- ResultsDBAny.hpp
- ResultsDBAny.cpp

14.231 ResultsDBBase Class Reference

Inheritance diagram for ResultsDBBase:



Public Member Functions

- virtual void flush () const

  If supported, flush data to the database or disk.
- virtual void allocate_vector (const StrStrSizet &iterator_id, const StringArray &location, ResultsOutputType stored_type, const int &len, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray())=0

  Pre-allocate a vector and (optionally) attach dimension scales and attributes. Insert elements using insert_into(...)
- virtual void allocate_matrix (const StrStrSizet &iterator_id, const StringArray &location, ResultsOutputType stored_type, const int &num_rows, const int &num_cols, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray())=0

  Pre-allocate a matrix and (optionally) attach dimension scales and attributes. Insert rows or columns using insert_into(...)
- virtual void insert (const StrStrSizet &iterator_id, const StringArray &location, const boost::any &data, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray(), const bool &transpose=false)=0

  addition with dimension scales and attributes

- virtual void insert_into (const StrStrSizet &iterator_id, const StringArray &location, const boost::any &data, const int &index, const bool &row)=0

  Insert a row or column into a pre-allocated matrix.
- virtual void add_metadata_to_method (const StrStrSizet &iterator_id, const AttributeArray &attrs)=0

  Add key:value metadata to a method.
- virtual void add_metadata_to_execution (const StrStrSizet &iterator_id, const AttributeArray &attrs)=0

  Add key:value metadata to an execution.
- virtual void add_metadata_to_object (const StrStrSizet &iterator_id, const StringArray &location, const AttributeArray &attrs)=0

  Associate key:value metadata with the object at the location.
- virtual void add_metadata_to_study (const AttributeArray &attrs)=0

  Associate key:value metadata to the study.
- template<typename StoredType >
  void array_allocate (const StrStrSizet &iterator_id, const std::string &data_name, size_t array_size, const MetaDataType &metadata)

  allocate an entry with sized array of the StoredType, e.g., array across response functions or optimization results sets
- template<typename StoredType >
  void array_insert (const StrStrSizet &iterator_id, const std::string &data_name, size_t index, const StoredType &sent_data)

  insert sent_data in specified position in previously allocated array
- virtual void insert (const StrStrSizet &iterator_id, const std::string &data_name, const boost::any &result, const MetaDataType &metadata)=0

  record addition with metadata map

Protected Attributes

- std::map< ResultsKeyType, ResultsValueType > iteratorData

  core data storage (map from key to value type)

14.231.1 Detailed Description

Class: ResultsDBBase

Description: A map-based container to store DAKOTA Iterator results in underlying boost::anys, with optional metadata

14.231.2 Member Function Documentation

14.231.2.1 void array_insert (const StrStrSizet & *iterator_id,* const std::string & *data_name,* size_t *index,* const StoredType & *sent_data*)

insert sent_data in specified position in previously allocated array

insert requires previous allocation, and does not allow metadata update

References Dakota::abort_handler(), ResultsDBBase::iteratorData, and Dakota::make_key().

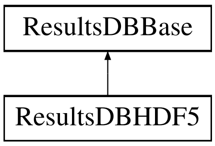
The documentation for this class was generated from the following file:

- ResultsDBBase.hpp

14.232 ResultsDBHDF5 Class Reference

Manage interactions between ResultsManager and the low-level HDFIOHelper class.

Inheritance diagram for ResultsDBHDF5:



Public Member Functions

- **ResultsDBHDF5** (bool in_core, std::shared_ptr< HDF5IOHelper > hdf5_helper_ptr)
- void flush () const override

  Flush HDF5 cache to disk.
- void allocate_vector (const StrStrSizet &iterator_id, const StringArray &location, ResultsOutputType stored_type, const int &len, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray()) override

  Pre-allocate a vector and (optionally) attach dimension scales and attributes. Insert elements using insert_into(...)
- void allocate_matrix (const StrStrSizet &iterator_id, const StringArray &location, ResultsOutputType stored_type, const int &num_rows, const int &num_cols, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray()) override

  Pre-allocate a matrix and (optionally) attach dimension scales and attributes. Insert rows or columns using insert_into(...)
- void insert_into (const StrStrSizet &iterator_id, const StringArray &location, const boost::any &data, const int &index, const bool &row) override

  Insert a row or column into a pre-allocated matrix.
- void insert (const StrStrSizet &iterator_id, const StringArray &location, const boost::any &data, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray(), const bool &transpose=false) override

  insert an arbitrary type (eg RealMatrix) with scales
- void add_metadata_to_method (const StrStrSizet &iterator_id, const AttributeArray &attrs) override

  Add attributes to the HDF5 method group.
- void add_metadata_to_execution (const StrStrSizet &iterator_id, const AttributeArray &attrs) override

  Add attributes to the HDF5 execution group.
- void add_metadata_to_object (const StrStrSizet &iterator_id, const StringArray &location, const AttributeArray &attrs) override

  Associate key:value metadata with the object at the location.
- void add_metadata_to_study (const AttributeArray &attrs) override

  Associate key:value metadata with the study.
- void insert (const StrStrSizet &iterator_id, const std::string &data_name, const boost::any &result, const MetaDataType &metadata) override

  record addition with metadata map
- template<typename StoredType >
  void array_allocate (const StrStrSizet &iterator_id, const std::string &data_name, size_t array_size, const MetaDataType &metadata)

  allocate an entry with sized array of the StoredType, e.g., array across response functions or optimization results sets
- template<typename StoredType >
  void **array_insert** (const StrStrSizet &iterator_id, const std::string &data_name, size_t index, const StoredType &stored_data)

Private Member Functions

- void attach_scales (const String &dset_name, const StrStrSizet &iterator_id, const StringArray &location, const DimScaleMap &scales)

  Attach a scale to a dataset.
- void add_attributes (const String &linkname, const AttributeArray &attrs)

  Add attributes to the object with linkname.
- void add_name_to_method (const StrStrSizet &iterator_id)

  Add the name (Dakota keyword) as metadata to a method group.
- bool method_in_cache (const StrStrSizet &iterator_id) const

  Check whether the name has already been added to a method group.

Private Attributes

- std::set< String > methodIdCache

  Cached method Ids; used to know which methods have already had their method_name attribute set. Hopefully faster than querying the HDF5 file.
- std::shared_ptr< HDF5IOHelper > hdf5Stream

  Instance of HDF5IOHelper (must be a pointer because it's shared with the global evaluation store instance.

Static Private Attributes

- static const std::string outputVersion = "2.1.0"

  Version of the output file. See comments near the definition in ResultsDBHDF5.cpp.

Additional Inherited Members

14.232.1 Detailed Description

Manage interactions between ResultsManager and the low-level HDFIOHelper class.

The documentation for this class was generated from the following files:

- ResultsDBHDF5.hpp
- ResultsDBHDF5.cpp

14.233 ResultsEntry< StoredType > Class Template Reference

Class to manage in-core vs. file database lookups.

Public Member Functions

- ResultsEntry (const ResultsManager &results_mgr, const StrStrSizet &iterator_id, const std::string &data_-name)

  Construct ResultsEntry containing retrieved item of StoredType.
- ResultsEntry (const ResultsManager &results_mgr, const StrStrSizet &iterator_id, const std::string &data_-name, size_t array_index)

  Construct ResultsEntry to retrieve item array_index from array of StoredType.

Private Member Functions

- ResultsEntry ()

  return a reference to the stored data, whether from core or file

Private Attributes

- bool coreActive

  whether the ResultsManager has an active in-core database
- StoredType dbData

  data retrieved from file data base
- const StoredType ∗ dbDataPtr

  non-const pointer to const data we don't own in the core case

14.233.1 Detailed Description

template<typename StoredType>class Dakota::ResultsEntry< StoredType >

Class to manage in-core vs. file database lookups.

ResultsEntry manages database lookups. If a core database is available, will return a reference directly to the stored data; if disk, will return reference to a local copy contained in this class. Allows disk-stored data to persist for minimum time during lookup to support true out-of-core use cases.

14.233.2 Constructor & Destructor Documentation

14.233.2.1 ResultsEntry ( ) [private]

return a reference to the stored data, whether from core or file

default construction disallowed: data must be initialized from DB lookup if needed

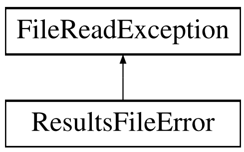
The documentation for this class was generated from the following file:

- ResultsManager.hpp

14.234 ResultsFileError Class Reference

exception throw for other results file read error

Inheritance diagram for ResultsFileError:



Public Member Functions

- **ResultsFileError** (const std::string &msg)

14.234.1 Detailed Description

exception throw for other results file read error

The documentation for this class was generated from the following file:

- dakota_global_defs.hpp

14.235 ResultsManager Class Reference

Results manager for iterator final data.

Public Member Functions

- ResultsManager ()

    default constructor: no databases active until they are added
- void clear_databases ()

    Delete all databases.
- void add_database (std::unique_ptr< ResultsDBBase >)

    Add a database.
- bool active () const

    whether any databases are active
- void flush () const

    Flush data to the database or disk, if supported.
- void close ()

    Close the database, if supported. This removes it from the active list of databases.
- template<typename StoredType >
void insert (const StrStrSizet &iterator_id, const StringArray &location, const StoredType &sent_data, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray(), const bool &transpose=false) const

    Insert using dimension scales and attributes (DimScaleMap and AttributeArray in dakota_results_types.hpp)
- void allocate_matrix (const StrStrSizet &iterator_id, const StringArray &location, ResultsOutputType stored_type, const int &num_rows, const int &num_cols, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray())

    Pre-allocate a matrix and (optionally) attach dimension scales and attributes. Insert rows or columns using insert_into(...)
- void allocate_vector (const StrStrSizet &iterator_id, const StringArray &location, ResultsOutputType stored_type, const int &len, const DimScaleMap &scales=DimScaleMap(), const AttributeArray &attrs=AttributeArray())

    Pre-allocate a vector and (optionally) attach dimension scales and attributes. Insert elements insert_into(...)
- template<typename StoredType >
void insert_into (const StrStrSizet &iterator_id, const StringArray &location, const StoredType &data, const int &index, const bool &row=true) const

    Insert a row or column into a matrix that was pre-allocated using allocate_matrix.
- void add_metadata_to_method (const StrStrSizet &iterator_id, const AttributeArray &attrs)

    Associate key:value metadata with all the results and executions of a method.
- void add_metadata_to_execution (const StrStrSizet &iterator_id, const AttributeArray &attrs)

    Associate key:value metadata with all the results for this execution of a method.
- void add_metadata_to_object (const StrStrSizet &iterator_id, const StringArray &location, const AttributeArray &attrs)

    Associate key:value metadata with the object at the location.
- void add_metadata_to_study (const AttributeArray &attrs)

Associate key:value metadata with the object at the location.

- template<typename StoredType >
void array_allocate (const StrStrSizet &iterator_id, const std::string &data_name, size_t array_size, const MetaDataType metadata=MetaDataType())

  allocate an entry with array of StoredType of array_size for future insertion; likely move to non-templated accessors for these
- template<typename StoredType >
void array_insert (const StrStrSizet &iterator_id, const std::string &data_name, size_t index, const StoredType &sent_data)

  insert into a previously allocated array of StoredType at index specified; metadata must be specified at allocation
- template<typename StoredType >
void array_insert (const StrStrSizet &iterator_id, const std::string &data_name, size_t index, StringMultiArrayConstView sent_data)

  specialization: insert a SMACV into a previously allocated array of StringArrayStoredType at index specified; metadata must be specified at allocation
- template<typename StoredType >
void insert (const StrStrSizet &iterator_id, const std::string &data_name, const StoredType &sent_data, const MetaDataType metadata=MetaDataType())

  insert data
- void **insert** (const StrStrSizet &iterator_id, const std::string &data_name, StringMultiArrayConstView sma_labels, const MetaDataType metadata=MetaDataType())

Public Attributes

- ResultsNames results_names

  Copy of valid results names for when manager is passed around.

Private Member Functions

- **ResultsManager** (const ResultsManager &)

Private Attributes

- std::vector< std::unique_ptr
< ResultsDBBase > > **resultsDBs**

Friends

- template<typename StoredType >
class ResultsEntry

  ResultsEntry is a friend of ResultsManager.

14.235.1 Detailed Description

Results manager for iterator final data.

The results manager provides the API for posting and retrieving iterator results data (and eventually run config/statistics). It can manage a set of underlying results databases, in or out of core, depending on configuration

The key for a results entry is documented in results_types.hpp, e.g., tuple<std::string, std::string, size_t, std::string>

For now, using concrete types for most insertion, since underlying databases like HDF5 might need concrete types; though template parameter for array allocation and retrieval.

All insertions overwrite any previous data.

The documentation for this class was generated from the following files:

- ResultsManager.hpp
- ResultsManager.cpp

14.236 ResultsNames Class Reference

List of valid names for iterator results.

Public Member Functions

- ResultsNames ()

    Default constructor.

Public Attributes

- size_t **namesVersion** = 0
- std::string **best_cv** = "Best Continuous Variables"
- std::string **best_div** = "Best Discrete Integer Variables"
- std::string **best_dsv** = "Best Discrete std::string Variables"
- std::string **best_drv** = "Best Discrete Real Variables"
- std::string **best_fns** = "Best Functions"
- std::string **moments_std** = "Moments: Standard"
- std::string **moments_central** = "Moments: Central"
- std::string **moments_std_num** = "Moments: Standard: Numerical"
- std::string **moments_central_num** = "Moments: Central: Numerical"
- std::string **moments_std_exp** = "Moments: Standard: Expansion"
- std::string **moments_central_exp** = "Moments: Central: Expansion"
- std::string **moment_cis** = "Moment Confidence Intervals"
- std::string **extreme_values** = "Extreme Values"
- std::string **map_resp_prob** = "Response to Probability Mapping"
- std::string **map_resp_rel** = "Response to Reliability Mapping"
- std::string **map_resp_genrel** = "Response to Generalized Reliability Mapping"
- std::string **map_prob_resp** = "Probability to Response Mapping"
- std::string **map_rel_resp** = "Reliability to Response Mapping"
- std::string **map_genrel_resp** = "Generalized Reliability to Response Mapping"
- std::string **pdf_histograms** = "PDF Histograms"
- std::string **correl_simple_all** = "Simple Correlations (All)"
- std::string **correl_simple_io** = "Simple Correlations (I/O)"
- std::string **correl_partial_io** = "Partial Correlations (I/O)"
- std::string **correl_simple_rank_all** = "Simple Rank Correlations (All)"
- std::string **correl_simple_rank_io** = "Simple Rank Correlations (I/O)"
- std::string **correl_partial_rank_io** = "Partial Rank Correlations (I/O)"
- std::string **pce_coeffs** = "PCE Coefficients: Standardized"
- std::string **pce_coeff_labels** = "PCE Coefficient Labels"
- std::string **cv_labels** = "Continuous Variable Labels"
- std::string **div_labels** = "Discrete Integer Variable Labels"
- std::string **dsv_labels** = "Discrete std::string Variable Labels"
- std::string **drv_labels** = "Discrete Real Variable Labels"
- std::string **fn_labels** = "Function Labels"

14.236.1 Detailed Description

List of valid names for iterator results.

All data in the ResultsNames class is public, basically just a struct

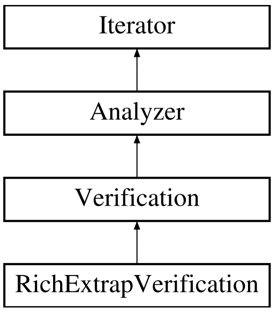
The documentation for this class was generated from the following file:

- ResultsManager.hpp

14.237 RichExtrapVerification Class Reference

Class for Richardson extrapolation for code and solution verification.

Inheritance diagram for RichExtrapVerification:



Public Member Functions

- RichExtrapVerification (ProblemDescDB &problem_db, Model &model)

    constructor
- ∼RichExtrapVerification ()

    destructor
- void core_run ()

    core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

    print the final iterator results

Private Member Functions

- void estimate_order ()

    perform a single estimation of convOrder using extrapolation()
- void converge_order ()

    iterate using extrapolation() until convOrder stabilizes
- void converge_qoi ()

    iterate using extrapolation() until QOIs stabilize
- void extrapolation (const RealVector &refine_triple, RealMatrix &qoi_triples)

    estimate convOrder from refinement and quantity of interest (QOI) triples
- void extrapolate_result (const RealVector &refine_triple, const RealMatrix &qoi_triples)

    predict the converged value based on the convergence rate and the value of Phi

Private Attributes

- unsigned short studyType

  internal code for extrapolation study type: SUBMETHOD_{CONVERGE_ORDER,CONVERGE_QOI,ESTIMATE_O-RDER}
- size_t numFactors

  number of refinement factors defined from active state variables
- RealVector initialCVars

  initial reference values for refinement factors
- size_t factorIndex

  the index of the active factor
- Real refinementRate

  rate of mesh refinement (default = 2.)
- RealMatrix convOrder

  the orders of convergence of the QOIs (numFunctions by numFactors)
- RealMatrix extrapQOI

  the extrapolated value of the QOI (numFunctions by numFactors)
- RealMatrix numErrorQOI

  the numerical uncertainty associated with level of refinement (numFunctions by numFactors)
- RealVector refinementRefPt

  This is a reference point reported for the converged extrapQOI and numErrorQOI. It currently corresponds to the coarsest mesh in the final refinement triple.

Additional Inherited Members

14.237.1 Detailed Description

Class for Richardson extrapolation for code and solution verification.

The RichExtrapVerification class contains several algorithms for performing Richardson extrapolation.

14.237.2 Member Function Documentation

14.237.2.1 void core_run ( ) [virtual]

core portion of run; implemented by all derived classes and may include pre/post steps in lieu of separate pre/post

Virtual run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from Iterator.

References Dakota::abort_handler(), Model::continuous_variables(), RichExtrapVerification::converge_order(), RichExtrapVerification::converge_qoi(), RichExtrapVerification::convOrder, RichExtrapVerification::estimate_-order(), RichExtrapVerification::extrapQOI, RichExtrapVerification::initialCVars, Iterator::iteratedModel, RichExtrap-Verification::numErrorQOI, RichExtrapVerification::numFactors, Analyzer::numFunctions, Iterator::outputLevel, RichExtrapVerification::refinementRefPt, and RichExtrapVerification::studyType.

14.237.2.2 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Verification.

References Model::continuous_variable_labels(), RichExtrapVerification::convOrder, Dakota::copy_data(), RichExtrapVerification::extrapQOI, Iterator::iteratedModel, RichExtrapVerification::numErrorQOI, Verification::print_results(), RichExtrapVerification::refinementRate, RichExtrapVerification::refinementRefPt, and Model::response_labels().

14.237.2.3 void estimate_order ( ) [private]

perform a single estimation of convOrder using extrapolation()

This algorithm executes a single refinement triple and returns convergence order estimates.

References RichExtrapVerification::extrapolate_result(), RichExtrapVerification::extrapolation(), RichExtrapVerification::extrapQOI, RichExtrapVerification::factorIndex, RichExtrapVerification::initialCVars, RichExtrapVerification::numErrorQOI, RichExtrapVerification::numFactors, Analyzer::numFunctions, RichExtrapVerification::refinementRate, and RichExtrapVerification::refinementRefPt.

Referenced by RichExtrapVerification::core_run().

14.237.2.4 void converge_order ( ) [private]

iterate using extrapolation() until convOrder stabilizes

This algorithm continues to refine until the convergence order estimate converges.

References Iterator::convergenceTol, RichExtrapVerification::convOrder, Dakota::copy_data(), RichExtrapVerification::extrapolate_result(), RichExtrapVerification::extrapolation(), RichExtrapVerification::extrapQOI, RichExtrapVerification::factorIndex, RichExtrapVerification::initialCVars, Iterator::maxIterations, RichExtrapVerification::numErrorQOI, RichExtrapVerification::numFactors, Analyzer::numFunctions, Iterator::outputLevel, RichExtrapVerification::refinementRate, and RichExtrapVerification::refinementRefPt.

Referenced by RichExtrapVerification::core_run().

14.237.2.5 void converge_qoi ( ) [private]

iterate using extrapolation() until QOIs stabilize

This algorithm continues to refine until the discretization error lies within a prescribed tolerance.

References Iterator::convergenceTol, RichExtrapVerification::extrapolate_result(), RichExtrapVerification::extrapolation(), RichExtrapVerification::extrapQOI, RichExtrapVerification::factorIndex, RichExtrapVerification::initialCVars, Iterator::maxIterations, RichExtrapVerification::numErrorQOI, RichExtrapVerification::numFactors, Analyzer::numFunctions, Iterator::outputLevel, RichExtrapVerification::refinementRate, and RichExtrapVerification::refinementRefPt.

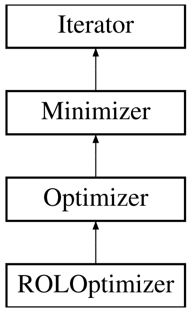
Referenced by RichExtrapVerification::core_run().

The documentation for this class was generated from the following files:

- RichExtrapVerification.hpp
- RichExtrapVerification.cpp

14.238 ROLOptimizer Class Reference

Inheritance diagram for ROLOptimizer:



Public Member Functions

- ROLOptimizer (ProblemDescDB &problem_db, Model &model)

  Standard constructor.
- ROLOptimizer (const String &method_name, Model &model)

  Alternate constructor for Iterator instantiations by name.
- ∼ROLOptimizer ()

  Destructor.
- void initialize_run () override

  Initializes the ROLOptimizer with values available after the chain of constructors has finished.
- void core_run () override

  Iterates the ROL solver to determine the optimal solution.
- void reset_solver_options (const Teuchos::ParameterList &)

  Support resetting ROL solver options.
- ROL::OptimizationProblem< Real > & get_rol_problem ()

  Accessor for the underlying ROL Problem.

Protected Member Functions

- void set_problem ()

  Helper function called during construction to extract problem information from the Model and set it for ROL.
- void set_rol_parameters ()

  Convenience function to map Dakota input and power-user parameters to ROL.

Protected Attributes

- Teuchos::ParameterList optSolverParams

  Parameters for the ROL::OptimizationSolver.
- unsigned short problemType

  ROL problem type.
- Teuchos::RCP< std::vector< Real > > rolX

  Handle to ROL's solution vector.
- Teuchos::RCP< ROL::StdVector
  < Real > > lowerBounds

  Handle to ROL's lower bounds vector.
- Teuchos::RCP< ROL::StdVector
  < Real > > upperBounds

  Handle to ROL's upper bounds vector.
- ROL::OptimizationProblem< Real > optProblem

  Handle to ROL::OptimizationProblem, part of ROL's simplified interface.

Additional Inherited Members

14.238.1 Detailed Description

ROLOptimizer specializes DakotaOptimizer to construct and run a ROL solver appropriate for the type of problem specified by the user.

14.238.2 Constructor & Destructor Documentation

14.238.2.1 ROLOptimizer (ProblemDescDB & *problem_db,* Model & *model*)

Standard constructor.

Implementation of ROLOptimizer class.

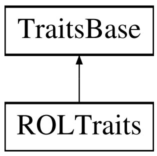
References ROLOptimizer::set_problem(), and ROLOptimizer::set_rol_parameters().

The documentation for this class was generated from the following files:

- ROLOptimizer.hpp
- ROLOptimizer.cpp

14.239 ROLTraits Class Reference

Inheritance diagram for ROLTraits:



Public Types

- typedef std::vector< Real > VecT

  ROL default data type to be used by Dakota data adapters.

Public Member Functions

- ROLTraits ()

  Default constructor.
- virtual ∼ROLTraits ()

  Destructor.
- bool supports_continuous_variables ()

  Return flag indicating ROL supports continuous variables.
- bool supports_linear_equality ()

  Return flag indicating ROL supports linear equalities.
- bool supports_linear_inequality ()

  Return flag indicating ROL supports linear inequalities.
- bool supports_nonlinear_equality ()

  Return flag indicating ROL supports nonlinear equalities.
- NONLINEAR_EQUALITY_FORMAT nonlinear_equality_format ()

Return ROL format for nonlinear equality constraints.

- bool supports_nonlinear_inequality ()

  Return flag indicating ROL supports nonlinear inequalities.

- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()

  Return ROL format for nonlinear inequality constraints.

14.239.1 Detailed Description

ROLTraits defines the types of problems and data formats ROL supports by overriding the default traits accessors in TraitsBase.

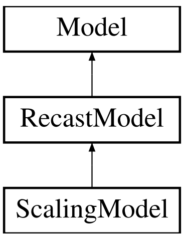
The documentation for this class was generated from the following file:

- ROLOptimizer.hpp

14.240 ScalingModel Class Reference

Scaling specialization of RecastModel.

Inheritance diagram for ScalingModel:



Public Member Functions

- ScalingModel (Model &sub_model)

  standard constructor

- ∼ScalingModel ()

  destructor

- RealVector cv_scaled2native (const RealVector &scaled_cv) const

Public members for help in final results recovery

- void resp_scaled2native (const Variables &native_vars, Response &updated_resp) const

  map responses from scaled to native space, updating provided Response in-place (on entry it's scaled response, on exit it's native)

- void secondary_resp_scaled2native (const RealVector &scaled_nln_cons, const ShortArray &asv, size_t num_native_primary, RealVector &native_fns) const

  Use scaled nonlinear constraints (sized total functions) to update the nonlinear constraints portion of the passed native_fns array.

- void response_modify_s2n (const Variables &native_vars, const Response &scaled_response, Response &native_response, int start_offset, int num_responses, bool response_unscale=true) const

  map responses from scaled to native space

- ActiveSet **default_active_set** ()

Protected Member Functions

- void assign_instance ()

  assign static pointer instance to this for use in static transformation functions
- void init_metadata () override

  default clear metadata in Recasts; derived classes can override to no-op
- bool update_variables_from_model (Model &model) override

  update active variables/bounds/labels from subModel
- void initialize_scaling (Model &sub_model)

  initialize scaling types, multipliers, and offsets; perform error checking
- void compute_scaling (int auto_type, int num_vars, RealVector &lbs, RealVector &ubs, RealVector &targets, const UShortArray &spec_types, const RealVector &scales, UShortArray &scale_types, RealVector &scale_-mults, RealVector &scale_offsets)

  general helper function for initializing scaling types and factors on a vector of variables, functions, constraints, etc.
- RealMatrix lin_coeffs_modify_n2s (const RealMatrix &native_coeffs, const RealVector &cv_multipliers, const RealVector &lin_multipliers) const

  general linear coefficients mapping from native to scaled space
- bool compute_scale_factor (const Real lower_bound, const Real upper_bound, Real ∗multiplier, Real ∗offset)

  automatically compute a single scaling factor – bounds case
- bool compute_scale_factor (const Real target, Real ∗multiplier)

  automatically compute a single scaling factor – target case
- void print_scaling (const String &info, const UShortArray &scale_types, const RealVector &scale_mults, const RealVector &scale_offsets, const StringArray &labels)

  print scaling information for a particular response type in tabular form
- bool need_resp_trans_byvars (const ShortArray &asv, int start_index, int num_resp) const

  determine if response transformation is needed due to variable transformations
- RealVector modify_n2s (const RealVector &native_vars, const UShortArray &scale_types, const RealVector &multipliers, const RealVector &offsets) const

  general RealVector mapping from native to scaled variables vectors:
- RealVector modify_s2n (const RealVector &scaled_vars, const UShortArray &scale_types, const RealVector &multipliers, const RealVector &offsets) const

  general RealVector mapping from scaled to native variables (and values)
- void response_modify_n2s (const Variables &scaled_vars, const Response &native_response, Response &scaled_response, int start_offset, int num_responses) const

  map reponses from native to scaled variable space

Static Protected Member Functions

- static bool scaling_active (const UShortArray &scale_types)

  check whether the passed scale types include any active (!= none) scale types
- static void variables_scaler (const Variables &scaled_vars, Variables &native_vars)

  RecastModel callback for variables scaling: transform variables from scaled to native (user) space.
- static void variables_unscaler (const Variables &native_vars, Variables &scaled_vars)

  RecastModel callback for inverse variables scaling: transform variables from native (user) to scaled space.
- static void primary_resp_scaler (const Variables &native_vars, const Variables &scaled_vars, const Response &native_response, Response &iterator_response)

  RecastModel callback for primary response scaling: transform responses (grads, Hessians) from native (user) to scaled space.
- static void secondary_resp_scaler (const Variables &native_vars, const Variables &scaled_vars, const Response &native_response, Response &scaled_response)

  RecastModel callback for secondary response scaling: transform constraints (grads, Hessians) from native (user) to scaled space.

Protected Attributes

- bool varsScaleFlag

  flag for variables scaling
- bool primaryRespScaleFlag

  flag for primary response scaling
- bool secondaryRespScaleFlag

  flag for secondary response scaling
- UShortArray cvScaleTypes

  scale flags for continuous vars.
- RealVector cvScaleMultipliers

  scales for continuous variables
- RealVector cvScaleOffsets

  offsets for continuous variables
- UShortArray responseScaleTypes

  scale flags for all responses
- RealVector responseScaleMultipliers

  scales for all responses
- RealVector responseScaleOffsets

  `offsets for all responses (zero`
  < for functions, not for nonlin con)
- UShortArray linearIneqScaleTypes

  scale flags for linear ineq
- RealVector linearIneqScaleMultipliers

  scales for linear ineq constrs.
- RealVector linearIneqScaleOffsets

  offsets for linear ineq constrs.
- UShortArray linearEqScaleTypes

  scale flags for linear eq.
- RealVector linearEqScaleMultipliers

  scales for linear constraints
- RealVector linearEqScaleOffsets

  offsets for linear constraints

Static Protected Attributes

- static ScalingModel * scaleModelInstance

  static pointer to this class for use in static callbacks

Additional Inherited Members

14.240.1 Detailed Description

Scaling specialization of RecastModel.

Specialization of RecastModel to scale Variables and/or Responses This class provides a simple constructor that forwards to the more complicated RecastModel API

14.240.2 Constructor & Destructor Documentation

14.240.2.1 ScalingModel (Model & *sub_model*)

standard constructor

This constructor computes various indices and mappings, then updates the properties of the RecastModel

References Model::cv(), ScalingOptions::cvScaleTypes, ScalingModel::cvScaleTypes, Model::div(), Model::drv(), Model::dsv(), RecastModel::init_maps(), ScalingModel::initialize_scaling(), RecastModel::inverse_mappings(), Model::modelId, Model::multivariate_distribution(), Model::mvDist, Model::num_primary_fns(), Model::num_secondary_fns(), Model::outputLevel, ScalingModel::primary_resp_scaler(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), ScalingModel::primaryRespScaleFlag, RecastModel::recast_model_id(), ScalingModel::responseScaleTypes, RecastModel::root_model_id(), ScalingModel::scaling_active(), Model::scalingOpts, ScalingModel::secondary_resp_scaler(), ScalingModel::secondaryRespScaleFlag, RecastModel::subModel, ScalingModel::variables_scaler(), ScalingModel::variables_unscaler(), and ScalingModel::varsScaleFlag.

14.240.3 Member Function Documentation

14.240.3.1 RealVector cv_scaled2native (const RealVector & *scaled_cv*) const

Public members for help in final results recovery

recover native variable values from the scaled space

Since this convenience function is public, it must have a fall-through to return a copy for when this scaling type isn't active.

References ScalingModel::cvScaleMultipliers, ScalingModel::cvScaleOffsets, ScalingModel::cvScaleTypes, ScalingModel::modify_s2n(), and ScalingModel::varsScaleFlag.

14.240.3.2 void resp_scaled2native (const Variables & *native_vars,* Response & *updated_resp*) const

map responses from scaled to native space, updating provided Response in-place (on entry it's scaled response, on exit it's native)

Since this convenience function is public, it must behave correctly when this scale type isn't active. It does, because it modifies in-place

References Response::active_set_request_vector(), Response::copy(), ScalingModel::need_resp_trans_byvars(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), ScalingModel::primaryRespScaleFlag, ScalingModel::response_modify_s2n(), ScalingModel::secondaryRespScaleFlag, and Response::update_partial().

Referenced by Optimizer::post_run().

14.240.3.3 void secondary_resp_scaled2native (const RealVector & *scaled_nln_cons,* const ShortArray & *asv,* size_t *num_native_primary,* RealVector & *native_fns*) const

Use scaled nonlinear constraints (sized total functions) to update the nonlinear constraints portion of the passed native_fns array.

Since this convenience function is public, it must have a fall-through to return a copy for when this scaling type isn't active.

scaled_nln_cons contains num_primary_fns(), followed by the nonlinear constraints to conditionally scale.

num_native_primary is the number of primary functions on the original user-provided Model, for example before data transformation, and is the starting index for populating nonlinear constraints in the native_fns vector.

References Dakota::copy_data_partial(), ScalingModel::modify_s2n(), ScalingModel::need_resp_trans_byvars(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), ScalingModel::responseScaleMultipliers, ScalingModel::responseScaleOffsets, ScalingModel::responseScaleTypes, and ScalingModel::secondaryRespScaleFlag.

14.240.3.4 void response_modify_s2n (const Variables & *native_vars,* const Response & *scaled_response,* Response & *native_response,* int *start_offset,* int *num_responses,* bool *unscale_resp* = `true`) const

map responses from scaled to native space

Unscaling response mapping: modifies response from scaled (iterator) to native (user) space. Maps num_responses starting at response_offset. If response_unscale = false, only variables will be unscaled, and responses left in scaled space.

References Response::active_set(), Variables::acv(), Variables::all_continuous_variable_ids(), Variables::all_continuous_variables(), Variables::continuous_variable_ids(), Variables::continuous_variables(), Dakota::copy_data(), Variables::cv(), ScalingModel::cvScaleMultipliers, ScalingModel::cvScaleOffsets, ScalingModel::cvScaleTypes, ActiveSet::derivative_vector(), Dakota::find_index(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian_view(), Response::function_hessians(), Response::function_labels(), Response::function_value(), Response::function_values(), Variables::icv(), Variables::inactive_continuous_variable_ids(), Variables::inactive_continuous_variables(), Model::num_primary_fns(), Model::outputLevel, ActiveSet::request_vector(), ScalingModel::responseScaleMultipliers, ScalingModel::responseScaleOffsets, ScalingModel::responseScaleTypes, Dakota::SCALING_LN_LOGBASE, Dakota::SCALING_LOGBASE, and Dakota::write_precision.

Referenced by LeastSq::get_confidence_intervals(), and ScalingModel::resp_scaled2native().

14.240.3.5 void initialize_scaling (Model & *sub_model*) `[protected]`

initialize scaling types, multipliers, and offsets; perform error checking

Initialize scaling types, multipliers, and offsets. Update the iteratedModel appropriately

References Dakota::abort_handler(), ScalingModel::compute_scaling(), Dakota::contains(), Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_variable_labels(), Model::continuous_variables(), Dakota::copy_data(), Model::cv(), ScalingModel::cvScaleMultipliers, ScalingModel::cvScaleOffsets, ScalingOptions::cvScales, ScalingOptions::cvScaleTypes, ScalingModel::cvScaleTypes, ScalingModel::lin_coeffs_modify_n2s(), Model::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_targets(), Model::linear_ineq_constraint_coeffs(), Model::linear_ineq_constraint_lower_bounds(), Model::linear_ineq_constraint_upper_bounds(), ScalingModel::linearEqScaleMultipliers, ScalingModel::linearEqScaleOffsets, ScalingModel::linearEqScaleTypes, ScalingModel::linearIneqScaleMultipliers, ScalingModel::linearIneqScaleOffsets, ScalingModel::linearIneqScaleTypes, ScalingOptions::linEqScales, ScalingOptions::linEqScaleTypes, ScalingOptions::linIneqScales, ScalingOptions::linIneqScaleTypes, ScalingModel::modify_n2s(), ScalingOptions::nlnEqScales, ScalingOptions::nlnEqScaleTypes, ScalingOptions::nlnIneqScales, ScalingOptions::nlnIneqScaleTypes, Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Model::num_linear_eq_constraints(), Model::num_linear_ineq_constraints(), Model::num_nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), Model::numFns, Model::outputLevel, ScalingModel::primaryRespScaleFlag, ScalingModel::print_scaling(), ScalingOptions::priScales, ScalingOptions::priScaleTypes, Model::response_labels(), ScalingModel::responseScaleMultipliers, ScalingModel::responseScaleOffsets, ScalingModel::responseScaleTypes, ScalingModel::scaling_active(), Model::scalingOpts, ScalingModel::secondaryRespScaleFlag, Model::supports_derivative_estimation(), Model::supportsEstimDerivs, and ScalingModel::varsScaleFlag.

Referenced by ScalingModel::ScalingModel(), and ScalingModel::update_variables_from_model().

14.240.3.6 RealMatrix lin_coeffs_modify_n2s (const RealMatrix & *src_coeffs,* const RealVector & *cv_multipliers,* const RealVector & *lin_multipliers*) const `[protected]`

general linear coefficients mapping from native to scaled space compute scaled linear constraint matrix given design variable multipliers and linear scaling multipliers. Only scales components corresponding to continuous variables so for src_coeffs of size MxN, lin_multipliers.size() <= M, cv_-multipliers.size() <= N

Referenced by ScalingModel::initialize_scaling().

14.240.3.7 void variables_scaler (const Variables & *scaled_vars,* Variables & *native_vars*) [static], [protected]

RecastModel callback for variables scaling: transform variables from scaled to native (user) space.

Variables map from iterator/scaled space to user/native space using a RecastModel.

References Variables::continuous_variable_labels(), Variables::continuous_variables(), ScalingModel::cvScale-Multipliers, ScalingModel::cvScaleOffsets, ScalingModel::cvScaleTypes, Variables::discrete_int_variables(), Variables::discrete_real_variables(), Variables::discrete_string_variables(), ScalingModel::modify_s2n(), Model-::outputLevel, ScalingModel::scaleModelInstance, and ScalingModel::varsScaleFlag.

Referenced by ScalingModel::ScalingModel().

14.240.3.8 void secondary_resp_scaler (const Variables & *native_vars,* const Variables & *scaled_vars,* const Response & *native_response,* Response & *iterator_response*) [static], [protected]

RecastModel callback for secondary response scaling: transform constraints (grads, Hessians) from native (user) to scaled space.

Constraint function map from user/native space to iterator/scaled/combined space using a RecastModel.

References Response::active_set_request_vector(), ScalingModel::need_resp_trans_byvars(), Model::num_-nonlinear_eq_constraints(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), Model::output-Level, ScalingModel::response_modify_n2s(), ScalingModel::scaleModelInstance, ScalingModel::secondaryResp-ScaleFlag, and Response::update_partial().

Referenced by ScalingModel::ScalingModel().

14.240.3.9 bool need_resp_trans_byvars (const ShortArray & *asv,* int *start_index,* int *num_resp*) const [protected]

determine if response transformation is needed due to variable transformations

Determine if variable transformations present and derivatives requested, which implies a response transformation is necessay

References ScalingModel::varsScaleFlag.

Referenced by ScalingModel::primary_resp_scaler(), ScalingModel::resp_scaled2native(), ScalingModel-::secondary_resp_scaled2native(), and ScalingModel::secondary_resp_scaler().

14.240.3.10 RealVector modify_n2s (const RealVector & *native_vars,* const UShortArray & *scale_types,* const RealVector & *multipliers,* const RealVector & *offsets*) const [protected]

general RealVector mapping from native to scaled variables vectors:

general RealVector mapping from native to scaled variables; loosely, in greatest generality: scaled_var = log((native_var - offset) / multiplier)

References Dakota::SCALING_LN_LOGBASE.

Referenced by ScalingModel::initialize_scaling(), and ScalingModel::variables_unscaler().

14.240.3.11 RealVector modify_s2n (const RealVector & *scaled_vars*, const UShortArray & *scale_types*, const RealVector & *multipliers*, const RealVector & *offsets*) const [protected]

general RealVector mapping from scaled to native variables (and values)

general RealVector mapping from scaled to native variables and/or vals; loosely, in greatest generality: scaled_var = (LOG_BASE^scaled_var) ∗ multiplier + offset

References Dakota::SCALING_LOGBASE.

Referenced by ScalingModel::cv_scaled2native(), ScalingModel::secondary_resp_scaled2native(), and ScalingModel::variables_scaler().

14.240.3.12 void response_modify_n2s (const Variables & *native_vars*, const Response & *native_response*, Response & *recast_response*, int *start_offset*, int *num_responses*) const [protected]

map reponses from native to scaled variable space

Scaling response mapping: modifies response from a model (user/native) for use in iterators (scaled). Maps num_-responses starting at response_offset

References Response::active_set(), Variables::acv(), Variables::all_continuous_variable_ids(), Variables::all_-continuous_variables(), Variables::continuous_variable_ids(), Variables::continuous_variables(), Dakota::copy_-data(), Variables::cv(), ScalingModel::cvScaleMultipliers, ScalingModel::cvScaleOffsets, ScalingModel::cvScale-Types, ActiveSet::derivative_vector(), Dakota::find_index(), Response::function_gradient_view(), Response-::function_gradients(), Response::function_hessian_view(), Response::function_hessians(), Response::function_-labels(), Response::function_value(), Response::function_values(), Variables::icv(), Variables::inactive_continuous-_variable_ids(), Variables::inactive_continuous_variables(), Model::num_primary_fns(), Model::outputLevel, Active-Set::request_vector(), ScalingModel::responseScaleMultipliers, ScalingModel::responseScaleOffsets, Scaling-Model::responseScaleTypes, Dakota::SCALING_LN_LOGBASE, and Dakota::write_precision.

Referenced by ScalingModel::primary_resp_scaler(), and ScalingModel::secondary_resp_scaler().

14.240.4 Member Data Documentation

14.240.4.1 ScalingModel ∗ scaleModelInstance [static], [protected]

static pointer to this class for use in static callbacks

initialization of static needed by RecastModel

Referenced by ScalingModel::assign_instance(), ScalingModel::primary_resp_scaler(), ScalingModel::secondary_-resp_scaler(), ScalingModel::variables_scaler(), and ScalingModel::variables_unscaler().

The documentation for this class was generated from the following files:

- ScalingModel.hpp
- ScalingModel.cpp

14.241 ScalingOptions Class Reference

Simple container for user-provided scaling data, possibly expanded by replicates through the models.

Public Member Functions

- ScalingOptions ()
  default ctor: no scaling specified
- ScalingOptions (const ProblemDescDB &problem_db, const SharedResponseData &srd)
  standard ctor: scaling from problem DB

Public Attributes

- UShortArray cvScaleTypes

    continuous variables scale types
- RealVector cvScales

    continuous variables scale values
- UShortArray priScaleTypes

    primary response scale types
- RealVector priScales

    primary response scale values
- UShortArray nlnIneqScaleTypes

    nonlinear inequality constraint scale types
- RealVector nlnIneqScales

    nonlinear inequality constraint scale values
- UShortArray nlnEqScaleTypes

    nonlinear equality constraint scale types
- RealVector nlnEqScales

    nonlinear equality constraint scale values
- UShortArray linIneqScaleTypes

    linear inequality constraint scale types
- RealVector linIneqScales

    linear inequality constraint scale values
- UShortArray linEqScaleTypes

    linear equality constraint scale types
- RealVector linEqScales

    linear equality constraint scale values

Static Private Member Functions

- static void default_scale_types (const RealVector &scale_values, UShortArray &scale_types)

    when values are given, but not types, initialize type to value
- static UShortArray scale_str2enum (const StringArray &scale_strs)

    convert problem DB strings to unsigned shorts

14.241.1 Detailed Description

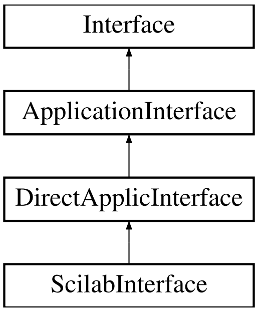
Simple container for user-provided scaling data, possibly expanded by replicates through the models.

The documentation for this class was generated from the following files:

- ScalingOptions.hpp
- ScalingOptions.cpp

14.242 ScilabInterface Class Reference

Inheritance diagram for ScilabInterface:



Public Member Functions

- ScilabInterface (const ProblemDescDB &problem_db)

    Constructor: start Scilab engine.
- ∼ScilabInterface ()

    Destructor: close Scilab engine.

Protected Member Functions

- virtual int derived_map_ac (const String &ac_name)

    execute an analysis code portion of a direct evaluation invocation
- int scilab_engine_run (const String &ac_name)

    principal Scilab execute function

Protected Attributes

- int scilabEngine

    identifier for the running Scilab enginer

14.242.1 Detailed Description

Specialization of DirectApplicInterface to link to Scilab analysis drivers. Includes convenience functions to map data to/from Scilab

The documentation for this class was generated from the following files:

- ScilabInterface.hpp
- ScilabInterface.cpp

14.243 SensAnalysisGlobal Class Reference

Class for a utility class containing correlation calculations and variance-based decomposition.

Public Member Functions

- SensAnalysisGlobal ()

    constructor
- ∼SensAnalysisGlobal ()

    destructor

- void compute_correlations (const VariablesArray &vars_samples, const IntResponseMap &resp_samples, const StringSetArray &dss_vals)

    computes four correlation matrices for input and output data simple, partial, simple rank, and partial rank
- void compute_correlations (const RealMatrix &vars_samples, const IntResponseMap &resp_samples)

    computes four correlation matrices for input and output data simple, partial, simple rank, and partial rank
- void archive_correlations (const StrStrSizet &run_identifier, ResultsManager &iterator_results, StringMultiArrayConstView cv_labels, StringMultiArrayConstView div_labels, StringMultiArrayConstView dsv_labels, StringMultiArrayConstView drv_labels, const StringArray &resp_labels, const size_t &inc_id=0) const

    save correlations to database
- bool correlations_computed () const

    returns corrComputed to indicate whether compute_correlations() has been invoked
- void print_correlations (std::ostream &s, StringMultiArrayConstView cv_labels, StringMultiArrayConstView div_labels, StringMultiArrayConstView dsv_labels, StringMultiArrayConstView drv_labels, const StringArray &resp_labels) const

    prints the correlations computed in compute_correlations()

Private Member Functions

- size_t find_valid_samples (const IntResponseMap &resp_samples, BoolDeque &valid_sample)

    find samples with finite response (any sample with any Nan or +/-Inf observation will be dropped)
- void valid_sample_matrix (const VariablesArray &vars_samples, const IntResponseMap &resp_samples, const StringSetArray &dss_vals, const BoolDeque is_valid_sample, RealMatrix &valid_data)

    extract a compact valid sample (vars/resp) matrix from the passed data
- void valid_sample_matrix (const RealMatrix &vars_samples, const IntResponseMap &resp_samples, const BoolDeque is_valid_sample, RealMatrix &valid_samples)

    extract a compact valid sample (vars/resp) matrix from the passed data
- void values_to_ranks (RealMatrix &valid_data)

    replace sample values with their ranks, in-place
- void center_rows (RealMatrix &data_matrix)

    center the passed matrix by its mean, in-place
- void correl_adjust (Real &corr_value)

    if result was NaN/Inf, preserve it, otherwise truncate to [-1.0, 1.0]
- void simple_corr (RealMatrix &total_data, const int &num_in, RealMatrix &corr_matrix)

    computes simple correlations, populating corr_matrix
- void partial_corr (RealMatrix &total_data, const int num_in, const RealMatrix &simple_corr_mat, RealMatrix &corr_matrix, bool &numerical_issues)

    computes partial correlations, populating corr_matrix and numerical_issues
- bool has_nan_or_inf (const RealMatrix &corr) const

    Return true if there are any NaN or Inf entries in the matrix.

Static Private Member Functions

- static bool rank_sort (const int &x, const int &y)

    sort algorithm to compute ranks for rank correlations

Private Attributes

- RealMatrix simpleCorr

    matrix to hold simple raw correlations
- RealMatrix simpleRankCorr

    matrix to hold simple rank correlations

- RealMatrix partialCorr

    matrix to hold partial raw correlations
- RealMatrix partialRankCorr

    matrix to hold partial rank correlations
- size_t numFns

    number of responses
- size_t numVars

    number of inputs
- bool numericalIssuesRaw

    flag indicating numerical issues in partial raw correlation calculations
- bool numericalIssuesRank

    flag indicating numerical issues in partial rank correlation calculations
- bool corrComputed

    flag indictaing whether correlations have been computed

Static Private Attributes

- static RealArray rawData = RealArray()

    array to hold temporary data before sort

14.243.1 Detailed Description

Class for a utility class containing correlation calculations and variance-based decomposition.

This class provides code for several of the sampling methods both in the NonD branch and in the PStudyDAC-E branch. Currently, the utility functions provide global sensitivity analysis through correlation calculations (e.g. simple, partial, rank, raw) as well as variance-based decomposition.

14.243.2 Member Function Documentation

14.243.2.1 void compute_correlations (const VariablesArray & *vars_samples,* const IntResponseMap & *resp_samples,* const StringSetArray & *dss_vals*)

computes four correlation matrices for input and output data simple, partial, simple rank, and partial rank

This version is used when full variables objects are being processed. Calculates simple correlation, partial correlation, simple rank correlation, and partial rank correlation coefficients.

References Dakota::abort_handler(), SensAnalysisGlobal::corrComputed, SensAnalysisGlobal::find_valid_-samples(), SensAnalysisGlobal::numericalIssuesRank, SensAnalysisGlobal::numericalIssuesRaw, SensAnalysis-Global::numFns, SensAnalysisGlobal::numVars, SensAnalysisGlobal::partial_corr(), SensAnalysisGlobal::partial-Corr, SensAnalysisGlobal::partialRankCorr, SensAnalysisGlobal::simple_corr(), SensAnalysisGlobal::simpleCorr, SensAnalysisGlobal::simpleRankCorr, SensAnalysisGlobal::valid_sample_matrix(), and SensAnalysisGlobal-::values_to_ranks().

Referenced by NonDSampling::compute_statistics(), ParamStudy::post_run(), FSUDesignCompExp::post_run(), and DDACEDesignCompExp::post_run().

14.243.2.2 void compute_correlations (const RealMatrix & *vars_samples,* const IntResponseMap & *resp_samples*)

computes four correlation matrices for input and output data simple, partial, simple rank, and partial rank

This version is used when compact samples matrix is being processed. Calculates simple correlation, partial correlation, simple rank correlation, and partial rank correlation coefficients.

References Dakota::abort_handler(), SensAnalysisGlobal::corrComputed, SensAnalysisGlobal::find_valid_-samples(), SensAnalysisGlobal::numericalIssuesRank, SensAnalysisGlobal::numericalIssuesRaw, SensAnalysis-Global::numFns, SensAnalysisGlobal::numVars, SensAnalysisGlobal::partial_corr(), SensAnalysisGlobal::partial-Corr, SensAnalysisGlobal::partialRankCorr, SensAnalysisGlobal::simple_corr(), SensAnalysisGlobal::simpleCorr, SensAnalysisGlobal::simpleRankCorr, SensAnalysisGlobal::valid_sample_matrix(), and SensAnalysisGlobal-::values_to_ranks().

14.243.2.3 void values_to_ranks (RealMatrix & *valid_data*) [private]

replace sample values with their ranks, in-place

When converting values to ranks, uses the average ranks of any tied values

Referenced by SensAnalysisGlobal::compute_correlations().

14.243.2.4 void simple_corr (RealMatrix & *total_data,* const int & *num_in,* RealMatrix & *corr_matrix*) [private]

computes simple correlations, populating corr_matrix

Calculates simple correlation coefficients from a matrix of data (oriented factors x observations):

- num_corr is number of rows of total data
- num_in indicates whether only pairs of correlations should be calculated between pairs of columns (num_in vs. num_corr-num_in); if num_in = num_corr, correlations are calculated between all columns

References SensAnalysisGlobal::center_rows(), and SensAnalysisGlobal::correl_adjust().

Referenced by SensAnalysisGlobal::compute_correlations().

14.243.2.5 void partial_corr (RealMatrix & *total_data,* const int *num_in,* const RealMatrix & *simple_corr_mat,* RealMatrix & *corr_matrix,* bool & *numerical_issues*) [private]

computes partial correlations, populating corr_matrix and numerical_issues

Calculates partial correlation coefficients between num_in inputs and numRows() - num_in outputs.

References Dakota::abort_handler(), SensAnalysisGlobal::center_rows(), SensAnalysisGlobal::correl_adjust(), Dakota::qr(), Dakota::qr_rsolve(), and Dakota::svd().

Referenced by SensAnalysisGlobal::compute_correlations().

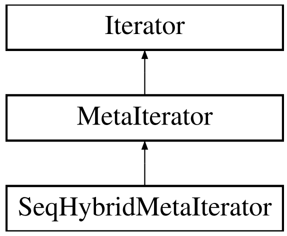
The documentation for this class was generated from the following files:

- SensAnalysisGlobal.hpp
- SensAnalysisGlobal.cpp

14.244 SeqHybridMetaIterator Class Reference

Method for sequential hybrid iteration using multiple optimization and nonlinear least squares methods on multiple models of varying fidelity.

Inheritance diagram for SeqHybridMetaIterator:



Public Member Functions

- SeqHybridMetaIterator (ProblemDescDB &problem_db)

  standard constructor
- SeqHybridMetaIterator (ProblemDescDB &problem_db, Model &model)

  alternate constructor
- ∼SeqHybridMetaIterator ()

  destructor

Protected Member Functions

- void core_run ()

  Performs the hybrid iteration by executing a sequence of iterators, using a similar sequence of models that may vary in fidelity.
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)

  print the final iterator results
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- IntIntPair estimate_partition_bounds ()

  estimate the minimum and maximum partition sizes that can be utilized by this Iterator
- const Variables & variables_results () const

  return the final solution from selectedIterators (variables)
- const Response & response_results () const

  return the final solution from selectedIterators (response)
- void initialize_iterator (int job_index)

  used by IteratorScheduler to set the starting data for a run
- void pack_parameters_buffer (MPIPackBuffer &send_buffer, int job_index)

  used by IteratorScheduler to pack starting data for an iterator run
- void unpack_parameters_initialize (MPIUnpackBuffer &recv_buffer, int job_index)

  used by IteratorScheduler to unpack starting data and initialize an iterator run
- void pack_results_buffer (MPIPackBuffer &send_buffer, int job_index)

  used by IteratorScheduler to pack results data from an iterator run
- void unpack_results_buffer (MPIUnpackBuffer &recv_buffer, int job_index)

  used by IteratorScheduler to unpack results data from an iterator run
- void update_local_results (int job_index)

  used by IteratorScheduler to update local results arrays
- void declare_sources ()

  Declare sources to the evaluations database.

Private Member Functions

- void run_sequential ()

  run a sequential hybrid
- void run_sequential_adaptive ()

  run a sequential adaptive hybrid
- void partition_sets (size_t num_sets, int job_index, size_t &start_index, size_t &job_size)

  convert num_sets and job_index into a start_index and job_size for extraction from parameterSets
- void extract_parameter_sets (int job_index, VariablesArray &partial_param_sets)

  extract partial_param_sets from parameterSets based on job_index
- void update_local_results (PRPArray &prp_results, int job_id)

  update the partial set of final results from the local iterator execution
- void initialize_iterator (const VariablesArray &param_sets)

  called by unpack_parameters_initialize(MPIUnpackBuffer) and initialize_iterator(int) to update the active Model and Iterator

Private Attributes

- String seqHybridType

  empty (default) or "adaptive"
- StringArray methodStrings

  the list of method pointer or method name identifiers
- StringArray modelStrings

  the list of model pointer identifiers for method identification by name
- bool lightwtMethodCtor

  use of lightweight Iterator construction by name
- bool singlePassedModel

  use of constructor that enforces use of a single passed Model
- IteratorArray selectedIterators

  the set of iterators, one for each entry in methodStrings
- ModelArray selectedModels

  the set of models, one for each iterator (if not lightweight construction)
- size_t seqCount

  hybrid sequence counter: 0 to numIterators-1
- Real progressThreshold

  when the progress metric falls below this threshold, the sequential adaptive hybrid switches to the next method
- PRP2DArray prpResults

  2-D array of results corresponding to numIteratorJobs, one set of results per job (iterators may return multiple final solutions)
- VariablesArray parameterSets

  1-D array of variable starting points for the iterator jobs

Friends

- class IteratorScheduler

  protect scheduler callback functions from general access

Additional Inherited Members

14.244.1 Detailed Description

Method for sequential hybrid iteration using multiple optimization and nonlinear least squares methods on multiple models of varying fidelity.

Sequential hybrid meta-iteration supports two approaches: (1) the non-adaptive sequential hybrid runs one method to completion, passes its best results as the starting point for a subsequent method, and continues this succession until all methods have been executed (the stopping rules are controlled internally by each iterator), and (2) the adaptive sequential hybrid uses adaptive stopping rules for the iterators that are controlled externally by this method. Any iterator may be used so long as it defines the notion of a final solution which can be passed as starting data for subsequent iterators.

14.244.2 Member Function Documentation

14.244.2.1 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Iterator.

References Response::function_values(), Response::is_null(), Variables::is_null(), MetaIterator::iterSched, Iterator-Scheduler::messagePass, and SeqHybridMetaIterator::prpResults.

14.244.2.2 void run_sequential ( ) [private]

run a sequential hybrid

In the sequential nonadaptive case, there is no interference with the iterators. Each runs until its own convergence criteria is satisfied. Status: fully operational.

References Iterator::accepts_multiple_points(), ParallelLibrary::bcast(), ParallelLibrary::bcast_hs(), Iterator-::initialize_graphics(), Model::interface_id(), Iterator::iteratedModel, IteratorScheduler::iterator_message_lengths(), IteratorScheduler::iteratorCommRank, IteratorScheduler::iteratorCommSize, IteratorScheduler::iteratorScheduling, IteratorScheduler::iteratorServerId, MetaIterator::iterSched, IteratorScheduler::messagePass, Iterator::methodPC-Iter, SeqHybridMetaIterator::methodStrings, IteratorScheduler::miPLIndex, Iterator::num_final_solutions(), Iterator-Scheduler::numIteratorJobs, IteratorScheduler::numIteratorServers, SeqHybridMetaIterator::pack_parameters_-buffer(), Iterator::parallelLib, SeqHybridMetaIterator::parameterSets, SeqHybridMetaIterator::prpResults, Parallel-Library::recv(), Iterator::response_results(), IteratorScheduler::schedule_iterators(), SeqHybridMetaIterator-::selectedIterators, SeqHybridMetaIterator::selectedModels, ParallelLibrary::send(), SeqHybridMetaIterator::seq-Count, SeqHybridMetaIterator::singlePassedModel, MPIPackBuffer::size(), Iterator::summaryOutputFlag, and Iterator::variables_results().

Referenced by SeqHybridMetaIterator::core_run().

14.244.2.3 void run_sequential_adaptive ( ) [private]

run a sequential adaptive hybrid

In the sequential adaptive case, there is interference with the iterators through the use of the ++ overloaded operator. iterator++ runs the iterator for one cycle, after which a progress_metric is computed. This progress metric is used to dictate method switching instead of each iterator's internal convergence criteria. Status: incomplete.

References Iterator::finalize_run(), Iterator::initialize_graphics(), Iterator::initialize_run(), IteratorScheduler::iterator-CommRank, IteratorScheduler::iteratorServerId, MetaIterator::iterSched, SeqHybridMetaIterator::methodStrings, IteratorScheduler::numIteratorServers, SeqHybridMetaIterator::progressThreshold, Iterator::response_results(), SeqHybridMetaIterator::selectedIterators, SeqHybridMetaIterator::selectedModels, SeqHybridMetaIterator::seqCount, Iterator::summaryOutputFlag, and Iterator::variables_results().

Referenced by SeqHybridMetaIterator::core_run().

14.244.2.4 void extract_parameter_sets (int *job_index,* VariablesArray & *partial_param_sets*) [inline], [private]

extract partial_param_sets from parameterSets based on job_index

This convenience function is executed on an iterator master (static scheduling) or a meta-iterator master (self scheduling) at run initialization time and has access to the full parameterSets array (this is All-Reduced for all peers at the completion of each cycle in run_sequential()).

References SeqHybridMetaIterator::parameterSets, and SeqHybridMetaIterator::partition_sets().

Referenced by SeqHybridMetaIterator::initialize_iterator(), and SeqHybridMetaIterator::pack_parameters_buffer().

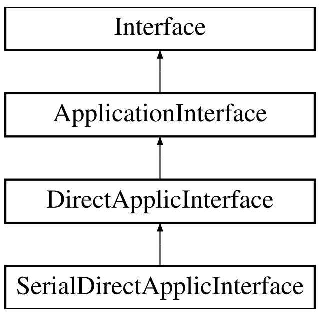
The documentation for this class was generated from the following files:

- SeqHybridMetaIterator.hpp
- SeqHybridMetaIterator.cpp

14.245 SerialDirectApplicInterface Class Reference

Sample derived interface class for testing serial simulator plug-ins using assign_rep().

Inheritance diagram for SerialDirectApplicInterface:



Public Member Functions

- SerialDirectApplicInterface (const Dakota::ProblemDescDB &problem_db)

  constructor
- ∼SerialDirectApplicInterface ()

  destructor

Protected Member Functions

- int derived_map_ac (const Dakota::String &ac_name)

  execute an analysis code portion of a direct evaluation invocation
- void derived_map_asynch (const Dakota::ParamResponsePair &pair)

  no-op hides base error; job batching occurs within wait_local_evaluations()
- void wait_local_evaluations (Dakota::PRPQueue &prp_queue)

  evaluate the batch of jobs contained in prp_queue

- void test_local_evaluations (Dakota::PRPQueue &prp_queue)

  invokes wait_local_evaluations() (no special nowait support)

- void set_communicators_checks (int max_eval_concurrency)

  no-op hides default run-time error checks at DirectApplicInterface level

Private Member Functions

- int rosenbrock (const Dakota::RealVector &c_vars, short asv, Dakota::Real &fn_val, Dakota::RealVector &fn-_grad, Dakota::RealSymMatrix &fn_hess)

  Rosenbrock plug-in test function.

Additional Inherited Members

14.245.1 Detailed Description

Sample derived interface class for testing serial simulator plug-ins using assign_rep().

The plug-in SerialDirectApplicInterface resides in namespace SIM and uses a copy of rosenbrock() to perform serial parameter to response mappings. It is used to demonstrate plugging in a serial direct analysis driver into Dakota in library mode. Test input files can then use an analysis_driver of "plugin_rosenbrock".

14.245.2 Member Function Documentation

14.245.2.1 void test_local_evaluations (Dakota::PRPQueue & *prp_queue*) [inline], [protected]

invokes wait_local_evaluations() (no special nowait support)

For use by ApplicationInterface::serve_evaluations_asynch(), which can provide a batch processing capability within message passing schedulers (called using chain IteratorScheduler::run_iterator() –> Model::serve() –> ApplicationInterface::serve_evaluations() –> ApplicationInterface::serve_evaluations_asynch()).

References SerialDirectApplicInterface::wait_local_evaluations().

The documentation for this class was generated from the following files:

- PluginSerialDirectApplicInterface.hpp
- PluginSerialDirectApplicInterface.cpp

14.246 TrackerHTTP::Server Struct Reference

struct to hold tracker/proxy pairs

Public Member Functions

- **Server** (std::string t, std::string p)

Public Attributes

- std::string **tracker**
- std::string **proxy**

14.246.1 Detailed Description

struct to hold tracker/proxy pairs

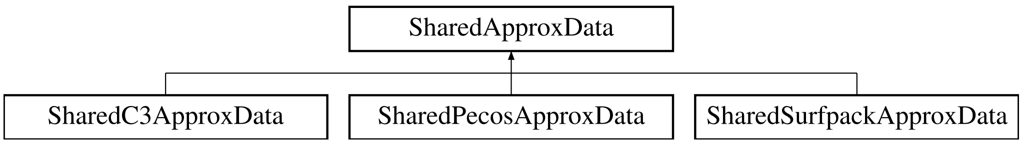
The documentation for this struct was generated from the following file:

- TrackerHTTP.hpp

14.247 SharedApproxData Class Reference

Base class for the shared approximation data class hierarchy.

Inheritance diagram for SharedApproxData:



Public Member Functions

- SharedApproxData ()

  default constructor
- SharedApproxData (ProblemDescDB &problem_db, size_t num_vars)

  standard constructor for envelope
- SharedApproxData (const String &approx_type, const UShortArray &approx_order, size_t num_vars, short data_order, short output_level)

  alternate constructor for envelope
- SharedApproxData (const SharedApproxData &approx)

  copy constructor
- virtual ∼SharedApproxData ()

  destructor
- SharedApproxData operator= (const SharedApproxData &approx)

  assignment operator
- virtual void active_model_key (const Pecos::ActiveKey &key)

  activate an approximation state based on its multi-index key
- virtual void clear_model_keys ()

  reset initial state by clearing all model keys for an approximation
- virtual void integration_iterator (const Iterator &iterator)

  set integration driver for structured grid approximations
- virtual short discrepancy_reduction () const

  return the discrepancy type for approximations that support MLMF
- virtual void build ()

  builds the shared approximation data from scratch
- virtual void rebuild ()

  rebuilds the shared approximation data incrementally
- virtual void pop (bool save_surr_data)

  back out the previous increment to the shared approximation data
- virtual bool push_available ()

  queries availability of pushing data associated with a trial set
- virtual size_t push_index (const Pecos::ActiveKey &key)

return index for restoring trial set within stored data sets

- virtual void pre_push ()

  push a previous state of the shared approximation data
- virtual void post_push ()

  clean up popped bookkeeping following push
- virtual size_t finalize_index (size_t i, const Pecos::ActiveKey &key)

  return index of i-th trial set within restorable bookkeeping sets
- virtual void pre_finalize ()

  finalize the shared approximation data following a set of increments
- virtual void post_finalize ()

  clean up popped bookkeeping following aggregation
- virtual void clear_inactive ()

  clear inactive approximation data
- virtual void pre_combine ()

  aggregate the shared approximation data from current and stored states
- virtual void post_combine ()

  clean up stored data sets after aggregation
- virtual void combined_to_active (bool clear_combined=true)

  promote aggregated data sets to active state
- virtual bool advancement_available ()

  queries availability of advancing the approximation resolution
- virtual void increment_order ()

  increments polynomial expansion order (PCE, FT)
- virtual void decrement_order ()

  decrements polynomial expansion order (PCE, FT)
- virtual void construct_basis (const Pecos::MultivariateDistribution &mv_dist)

  construct the shared basis for an expansion-based approximation
- virtual void update_basis_distribution_parameters (const Pecos::MultivariateDistribution &mvd)

  propagate updates to random variable distribution parameters to a polynomial basis
- virtual void configuration_options (const Pecos::ExpansionConfigOptions &ec_options)

  set ExpansionConfigOptions instance as a group specification
- virtual void configuration_options (const Pecos::BasisConfigOptions &bc_options)

  set BasisConfigOptions instance as a group specification
- virtual void configuration_options (const Pecos::RegressionConfigOptions &rc_options)

  set BasisConfigOptions instance as a group specification
- virtual void random_variables_key (const BitArray &random_vars_key)

  assign key identifying a subset of variables that are to be treated as random for statistical purposes (e.g. expectation)
- virtual void refinement_statistics_mode (short stats_mode)

  assign mode for statistics roll-up: {ACTIVE,COMBINED}_EXPANSION_STATS
- virtual const
  Pecos::BitArrayULongMap & sobol_index_map () const

  return set of Sobol indices that have been requested (e.g., as constrained by throttling) and are computable by a (sparse) expansion of limited order
- const Pecos::ActiveKey & active_model_key () const

  return active multi-index key
- bool formulation_updated () const

  query whether the form of an approximation has been updated
- void formulation_updated (bool update)

  assign the status of approximation formulation updates
- void set_bounds (const RealVector &c_l_bnds, const RealVector &c_u_bnds, const IntVector &di_l_bnds, const IntVector &di_u_bnds, const RealVector &dr_l_bnds, const RealVector &dr_u_bnds)

set approximation lower and upper bounds (currently only used by graphics)
- std::shared_ptr< SharedApproxData > data_rep () const

  returns dataRep for access to derived class member functions that are not mapped to the top SharedApproxData level

Protected Member Functions

- SharedApproxData (BaseConstructor, ProblemDescDB &problem_db, size_t num_vars)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- SharedApproxData (NoDBBaseConstructor, const String &approx_type, size_t num_vars, short data_order, short output_level)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

Protected Attributes

- size_t numVars

  number of variables in the approximation
- String approxType

  approximation type identifier
- short buildDataOrder

  order of the data used for surrogate construction, in ActiveSet request vector 3-bit format.
- short outputLevel

  output verbosity level: {SILENT,QUIET,NORMAL,VERBOSE,DEBUG}_OUTPUT
- Pecos::ActiveKey activeKey

  key indicating the active model or model-pair used for approximation data
- String modelExportPrefix

  Prefix for model export files.
- unsigned short modelExportFormat

  Bitmapped format request for exported models.
- RealVector approxCLowerBnds

  approximation continuous lower bounds (used by 3D graphics and Surfpack KrigingModel)
- RealVector approxCUpperBnds

  approximation continuous upper bounds (used by 3D graphics and Surfpack KrigingModel)
- IntVector approxDILowerBnds

  approximation continuous lower bounds
- IntVector approxDIUpperBnds

  approximation continuous upper bounds
- RealVector approxDRLowerBnds

  approximation continuous lower bounds
- RealVector approxDRUpperBnds

  approximation continuous upper bounds
- std::map< Pecos::ActiveKey, bool > formUpdated

  tracker for changes in order,rank configuration since last build (used by DataFitSurrModel::rebuild_approximation())

Private Member Functions

- std::shared_ptr< SharedApproxData > get_shared_data (ProblemDescDB &problem_db, size_t num_vars)

  Used only by the standard envelope constructor to initialize dataRep to the appropriate derived type.
- std::shared_ptr< SharedApproxData > get_shared_data (const String &approx_type, const UShortArray &approx_order, size_t num_vars, short data_order, short output_level)

  Used only by the alternate envelope constructor to initialize dataRep to the appropriate derived type.

Private Attributes

- std::shared_ptr< SharedApproxData > dataRep

    pointer to the letter (initialized only for the envelope)

Friends

- class **Approximation**
- class **TaylorApproximation**
- class **TANA3Approximation**
- class **QMEApproximation**
- class **GaussProcApproximation**
- class **VPSApproximation**
- class **PecosApproximation**
- class **C3Approximation**
- class **SurfpackApproximation**
- class **SurrogatesGPApprox**
- class **SurrogatesBaseApprox**
- class **SurrogatesPolyApprox**

14.247.1 Detailed Description

Base class for the shared approximation data class hierarchy.

The SharedApproxData class is the base class for the shared approximation data class hierarchy in DAKOTA. For memory efficiency and enhanced polymorphism, the approximation hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (SharedApproxData) serves as the envelope and one of the derived classes (selected in SharedApproxData::get_shared_data()) serves as the letter.

14.247.2 Constructor & Destructor Documentation

14.247.2.1 SharedApproxData ( )

default constructor

For the default constructor, dataRep is NULL.

Referenced by SharedApproxData::get_shared_data().

14.247.2.2 SharedApproxData (ProblemDescDB & *problem_db*, size_t *num_vars*)

standard constructor for envelope

Envelope constructor only needs to extract enough data to properly execute get_shared_data, since SharedApprox-Data(BaseConstructor, problem_db) builds the actual base class data for the derived approximations.

References Dakota::abort_handler(), and SharedApproxData::dataRep.

14.247.2.3 SharedApproxData (const String & *approx_type*, const UShortArray & *approx_order*, size_t *num_vars*, short *data_order*, short *output_level*)

alternate constructor for envelope

This is the alternate envelope constructor for instantiations on the fly. Since it does not have access to problem_db, it utilizes the NoDBBaseConstructor constructor chain.

References Dakota::abort_handler(), and SharedApproxData::dataRep.

14.247.2.4 SharedApproxData (const SharedApproxData & *shared_data*)

copy constructor

Copy constructor manages sharing of dataRep.

14.247.2.5 SharedApproxData (BaseConstructor , ProblemDescDB & *problem_db*, size_t *num_vars*) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_shared_data() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_shared_data() again). Since the letter IS the representation, its rep pointer is set to NULL (an uninitialized pointer causes problems in ∼SharedApproxData).

References SharedApproxData::approxType, SharedApproxData::buildDataOrder, ProblemDescDB::get_bool(), ProblemDescDB::get_db_model_node(), ProblemDescDB::get_string(), ProblemDescDB::set_db_model_nodes(), Dakota::strbegins(), and Dakota::strends().

14.247.2.6 SharedApproxData (NoDBBaseConstructor , const String & *approx_type*, size_t *num_vars*, short *data_order*, short *output_level*) [protected]

constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)

This constructor is the one which must build the base class data for all derived classes. get_shared_data() instantiates a derived class letter and the derived constructor selects this base class constructor in its initialization list (to avoid recursion in the base class constructor calling get_shared_data() again). Since the letter IS the representation, its rep pointer is set to NULL (an uninitialized pointer causes problems in ∼SharedApproxData).

References SharedApproxData::approxType, SharedApproxData::buildDataOrder, Dakota::strbegins(), and Dakota::strends().

14.247.3 Member Function Documentation

14.247.3.1 std::shared_ptr< SharedApproxData > get_shared_data (ProblemDescDB & *problem_db*, size_t *num_vars*) [private]

Used only by the standard envelope constructor to initialize dataRep to the appropriate derived type.

Used only by the envelope constructor to initialize dataRep to the appropriate derived type.

References ProblemDescDB::get_string(), SharedApproxData::SharedApproxData(), and Dakota::strends().

14.247.3.2 std::shared_ptr< SharedApproxData > get_shared_data (const String & *approx_type*, const UShortArray & *approx_order*, size_t *num_vars*, short *data_order*, short *output_level*) [private]

Used only by the alternate envelope constructor to initialize dataRep to the appropriate derived type.

Used only by the envelope constructor to initialize dataRep to the appropriate derived type.

References SharedApproxData::SharedApproxData(), and Dakota::strends().

14.247.4 Member Data Documentation

14.247.4.1 short buildDataOrder [protected]

order of the data used for surrogate construction, in ActiveSet request vector 3-bit format.

This setting distinguishes derivative data intended for use in construction (includes derivatives w.r.t. the build variables) from derivative data that may be approximated separately (excludes derivatives w.r.t. auxilliary variables). This setting should also not be inferred directly from the responses specification, since we may need gradient support for evaluating gradients at a single point (e.g., the center of a trust region), but not require gradient evaluations at every point.

Referenced by SharedSurfpackApproxData::add_sd_to_surfdata(), SharedApproxData::SharedApproxData(), and SharedPecosApproxData::SharedPecosApproxData().

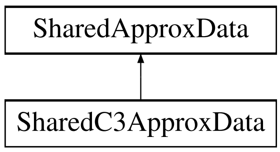
The documentation for this class was generated from the following files:

- SharedApproxData.hpp
- SharedApproxData.cpp

14.248 SharedC3ApproxData Class Reference

Derived approximation class for global basis polynomials.

Inheritance diagram for SharedC3ApproxData:



Public Member Functions

- SharedC3ApproxData ()
  default constructor
- SharedC3ApproxData (ProblemDescDB &problem_db, size_t num_vars)
  standard ProblemDescDB-driven constructor
- SharedC3ApproxData (const String &approx_type, const UShortArray &approx_order, size_t num_vars, short data_order, short output_level)
  on-the-fly constructor (no problem DB)
- ∼SharedC3ApproxData ()
  destructor
- size_t regression_size ()
  return number of FT unknowns using start_rank(), max_rank(), start_orders(), max_order()
- size_t max_rank_regression_size ()
  return number of FT unknowns using maximum rank, start_orders(), max_order()
- size_t max_order_regression_size ()
  return number of FT unknowns using start_rank(), max_rank(), and maximum basis order
- size_t max_regression_size ()
  return number of FT unknowns using maxima for rank and basis order
- void set_parameter (String var, const UShortArray &val)
  set UShortArray attribute value based on identifier string
- void set_parameter (String var, unsigned short val)
  set unsigned short attribute value based on identifier string
- void set_parameter (String var, size_t val)

set size_t attribute value based on identifier string
- void set_parameter (String var, bool val)

  set bool attribute value based on identifier string
- void set_parameter (String var, short val)

  set short attribute value based on identifier string
- void set_parameter (String var, double val)

  set double attribute value based on identifier string
- void set_parameter (String var, int val)

  set int attribute value based on identifier string
- void set_active_parameter (String var, const UShortArray &val)

  set active UShortArray attribute value based on identifier string
- void set_active_parameter (String var, unsigned short val)

  set active unsigned short attribute value based on identifier string
- void set_active_parameter (String var, size_t val)

  set active size_t attribute value based on identifier string
- void set_active_parameter (String var, int val)

  set active int attribute value based on identifier string
- const UShortArray & start_orders () const

  return active start value for basis order
- UShortArray & start_orders ()

  return active start value for basis order (mutable)
- unsigned short max_order () const

  return active maximum value for basis order
- unsigned short & max_order ()

  return active maximum value for basis order (mutable)
- size_t start_rank () const

  return active start value for expansion rank
- size_t & start_rank ()

  return active start value for expansion rank (mutable)
- size_t max_rank () const

  return active maximum value for expansion rank
- size_t & max_rank ()

  return active maximum value for expansion rank (mutable)
- size_t max_cross_validation_rank_candidates () const

  return maxCVRankCandidates
- unsigned short max_cross_validation_order_candidates () const

  return maxCVOrderCandidates
- void **assign_start_ranks** (SizetVector &start_ranks) const
- void update_basis ()

  update oneApproxOpts with active basis orders after an order change
- void update_basis (const UShortArray &start_orders, unsigned short max_order)

  update oneApproxOpts with passed basis orders after an order change
- void update_basis (size_t v, unsigned short start_order, unsigned short max_order)

  update oneApproxOpts for variable v with passed basis orders

Static Public Member Functions

- static size_t regression_size (size_t num_v, size_t rank, size_t max_rank, const UShortArray &orders, unsigned short max_order)

  return number of FT unknowns given scalars: num vars, rank, order

Protected Member Functions

- void active_model_key (const Pecos::ActiveKey &key)
  activate an approximation state based on its multi-index key
- void construct_basis (const Pecos::MultivariateDistribution &mv_dist)
  construct the shared basis for an expansion-based approximation
- short discrepancy_reduction () const
  return the discrepancy type for approximations that support MLMF
- void random_variables_key (const BitArray &random_vars_key)
  assign key identifying a subset of variables that are to be treated as random for statistical purposes (e.g. expectation)
- void build ()
  builds the shared approximation data from scratch
- void increment_order ()
  increments polynomial expansion order (PCE, FT)
- void decrement_order ()
  decrements polynomial expansion order (PCE, FT)
- void pop (bool save_surr_data)
  back out the previous increment to the shared approximation data
- bool push_available ()
  queries availability of pushing data associated with a trial set
- size_t push_index (const Pecos::ActiveKey &key)
  return index for restoring trial set within stored data sets
- void post_push ()
  clean up popped bookkeeping following push
- void pre_combine ()
  aggregate the shared approximation data from current and stored states
- bool advancement_available ()
  queries availability of advancing the approximation resolution
- void **max_rank_advancement** (bool r_advance)
- void **max_order_advancement** (bool o_advance)
- bool **increment_max_rank** ()
- bool **increment_max_order** ()

Protected Attributes

- std::vector< OneApproxOpts * > oneApproxOpts
  one-D approximation options (basis type, poly order, etc.)
- MultiApproxOpts * multiApproxOpts
  n-D approximation options, augmenting one-D options
- bool respScaling
  option to scale response data prior to regression
- UShortArray startOrders
  starting user specification for polynomial orders (from start_order scalar plus anisotropic dimension preference)
- std::map< Pecos::ActiveKey,
  UShortArray > startOrdersMap
  starting values for polynomial order (prior to adaptive refinement); for each model key, there is an array of polynomial orders per variable
- unsigned short kickOrder
  user specification for increment in order used within adapt_order
- unsigned short maxOrder
  maximum value for polynomial order from user spec

- std::map< Pecos::ActiveKey, unsigned short > maxOrderMap

  user specification for maximum order used within adapt_order; usually a scalar specification but can be adapted per model key for MAX_{ORDER,RANK_ORDER}_ADVANCEMENT refine types
- bool adaptOrder

  C3 FT can support CV over polynomial order in addition to adapt_rank.
- UShortArray combinedOrders

  polynomial basis order for combined expansion for each variable core
- size_t startRank

  starting user specification for rank (not augmented by dimension preference); Note: rank sequence spec is managed externally and becomes reflected in startRank model index mapping
- std::map< Pecos::ActiveKey, size_t > startRankMap

  starting values for rank (note: adapt_rank currently covers refinement); for each model index key, there is a scalar starting rank (recovered rank in C3FnrainPtrs can vary per core/variable and per QoI)
- size_t kickRank

  user specification for increment in rank used within adapt_rank
- size_t maxRank

  scalar user specification for maximum allowable rank when adapting
- std::map< Pecos::ActiveKey, size_t > maxRankMap

  user specification for maximum rank used within adapt_rank; usually a scalar specification but can be adapted per model key for MAX_{RANK,RANK_ORDER}_ADVANCEMENT refine types
- bool adaptRank

  internal C3 adaptation that identifies the best rank representation for a set of sample data based on cross validation
- short regressType

  type of regression solver for forming FT approximation
- double regressRegParam

  penalty parameter if regularized regression
- double solverTol

  tolerance on regression solver
- double solverRoundingTol

  tolerance for rounding (performing a truncation operation on a FT expansion) within the regression solver
- double statsRoundingTol

  tolerance for rounding (performing a truncation operation on a FT expansion) when post-processing an expansion: computing products for moments, combining expansions with c3axpy, etc.
- size_t maxSolverIterations

  maximum number of iterations for regression solver
- int crossMaxIter

  maximum number of iterations for (future) cross iteration solver
- int randomSeed

  C3 regression solver employs a random seed.
- short combineType

  type of discrepancy calculation: additive, multiplicative, or both
- short discrepReduction

  type of multilevel discrepancy emulation: distinct or recursive
- short allocControl

  type of multilevel strategy for sample allocation: ESTIMATOR_VARIANCE, RANK_SAMPLING, GREEDY
- short c3AdvancementType

  type of advancement strategy used in uniform refinement: {START_ORDER,START_RANK,MAX_ORDER,MAX_RANK,MAX_RANK_ORDER}_ADVANCEMENT
- std::map< Pecos::ActiveKey, bool > c3MaxRankAdvance

flag indicating availability of rank advancement (accumulated from C3Approximation::advancement_available())

- std::map< Pecos::ActiveKey, bool > c3MaxOrderAdvance

  flag indicating availability of order advancement (accumulated from C3Approximation::advancement_available())

- unsigned short maxCVOrderCandidates

  restrict the number of candidates within cross validation for order (by increasing start order when needed as max order is advanced)

- size_t maxCVRankCandidates

  restrict the number of candidates within cross validation for rank (by increasing start rank when needed as max rank is advanced)

- SizetArray randomIndices

  indices for random subset when approximating in all-variables mode

- std::map< Pecos::ActiveKey,
  size_t > poppedCounts

  number of instances within the popped arrays (mostly a placeholder for supporting push_available())

Friends

- class **C3Approximation**

14.248.1 Detailed Description

Derived approximation class for global basis polynomials.

The SharedC3ApproxData class provides a global approximation based on basis polynomials. This includes orthogonal polynomials used for polynomial chaos expansions and interpolation polynomials used for stochastic collocation.

14.248.2 Member Function Documentation

14.248.2.1 size_t regression_size (size_t *num_v*, size_t *rank*, size_t *max_rank*, const UShortArray & *orders*, unsigned short *max_order*) [inline], [static]

return number of FT unknowns given scalars: num vars, rank, order

```
simplified estimation for scalar-valued rank and order (e.g., from
start rank/order user specification)
```

inline size_t SharedC3ApproxData:: regression_size(size_t num_v, size_t rank, size_t order) { Each dimension has its own rank within the product of function cores. This fn estimates for the case where rank and order are either constant across dimensions or averaged into a scalar.

> the first and last core contribute p∗r terms the middle cores contribute r∗r∗p terms

size_t p = order+1.; switch (num_v) { case 1: return p; break; // collapses to a 1D PCE case 2: return 2.∗p∗rank; break; // first and last core, no middle default: return p∗rank∗(2. + (num_v-2)∗rank); break; // first,last,middle } }simplified estimation for scalar-valued rank and vector-valued order (e.g., from start rank/start order/dimension pref user specification)

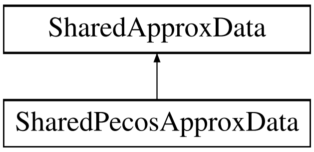
The documentation for this class was generated from the following files:

- SharedC3ApproxData.hpp
- SharedC3ApproxData.cpp

14.249 SharedPecosApproxData Class Reference

Derived approximation class for global basis polynomials.

Inheritance diagram for SharedPecosApproxData:



Public Member Functions

- SharedPecosApproxData ()

    default constructor
- SharedPecosApproxData (const String &approx_type, const UShortArray &approx_order, size_t num_vars, short data_order, short output_level)

    alternate constructor
- SharedPecosApproxData (ProblemDescDB &problem_db, size_t num_vars)

    standard ProblemDescDB-driven constructor
- ∼SharedPecosApproxData ()

    destructor
- void random_variables_key (const Pecos::BitArray &random_vars_key)

    set pecosBasisApprox.randomVarsKey
- void update_basis_distribution_parameters (const Pecos::MultivariateDistribution &u_dist)

    invoke Pecos::SharedPolyApproxData::update_basis_distribution_parameters()
- void polynomial_basis (const std::vector< Pecos::BasisPolynomial > &poly_basis)

    set Pecos::SharedOrthogPolyApproxData::polynomialBasis
- const std::vector
  < Pecos::BasisPolynomial > & polynomial_basis () const

    get Pecos::SharedOrthogPolyApproxData::polynomialBasis
- std::vector
  < Pecos::BasisPolynomial > & polynomial_basis ()

    get Pecos::SharedOrthogPolyApproxData::polynomialBasis
- void allocate (const UShort2DArray &mi)

    set Pecos::SharedOrthogPolyApproxData::multiIndex and allocate associated arrays
- const UShort2DArray & multi_index () const

    get active Pecos::SharedOrthogPolyApproxData::multiIndex
- const std::map
  < Pecos::ActiveKey,
  UShort2DArray > & multi_index_map () const

    get Pecos::SharedOrthogPolyApproxData::multiIndex
- const Pecos::BitArrayULongMap & sobol_index_map () const

    return Pecos::SharedPolyApproxData::sobolIndexMap
- void coefficients_norms_flag (bool flag)

    invoke Pecos::SharedOrthogPolyApproxData::coefficients_norms_flag()
- size_t expansion_terms () const

    return Pecos::SharedOrthogPolyApproxData::expansion_terms()
- const UShortArray & expansion_order () const

    return Pecos::SharedOrthogPolyApproxData::expansion_order()
- void expansion_order (const UShortArray &order)

invokes Pecos::SharedOrthogPolyApproxData::expansion_order(UShortArray&)
- void configuration_options (const Pecos::ExpansionConfigOptions &ec_options)

  set the expansion configuration options within Pecos::SharedPolyApproxData
- void configuration_options (const Pecos::BasisConfigOptions &bc_options)

  set the basis configuration options within Pecos::SharedPolyApproxData
- void configuration_options (const Pecos::RegressionConfigOptions &rc_options)

  set the regression configuration options within Pecos::SharedRegressOrthogPolyApproxData
- void refinement_statistics_mode (short stats_mode)

  update ExpansionConfigOptions::refineStatsType

Protected Member Functions

- void active_model_key (const Pecos::ActiveKey &key)

  activate an approximation state based on its multi-index key
- void clear_model_keys ()

  reset initial state by clearing all model keys for an approximation
- void construct_basis (const Pecos::MultivariateDistribution &mv_dist)

  construct the shared basis for an expansion-based approximation
- void integration_iterator (const Iterator &iterator)

  set integration driver for structured grid approximations
- short discrepancy_reduction () const

  return the discrepancy type for approximations that support MLMF
- void build ()

  builds the shared approximation data from scratch
- void rebuild ()

  rebuilds the shared approximation data incrementally
- void pop (bool save_surr_data)

  back out the previous increment to the shared approximation data
- bool push_available ()

  queries availability of pushing data associated with a trial set
- size_t push_index (const Pecos::ActiveKey &key)
- void pre_push ()

  push a previous state of the shared approximation data
- void post_push ()

  clean up popped bookkeeping following push
- size_t finalize_index (size_t i, const Pecos::ActiveKey &key)

  return index of i-th trial set within restorable bookkeeping sets
- void pre_finalize ()

  finalize the shared approximation data following a set of increments
- void post_finalize ()

  clean up popped bookkeeping following aggregation
- void pre_combine ()

  aggregate the shared approximation data from current and stored states
- void post_combine ()

  clean up stored data sets after aggregation
- void combined_to_active (bool clear_combined=true)

  promote aggregated data sets to active state
- bool advancement_available ()

  queries availability of advancing the approximation resolution
- void clear_inactive ()

clear inactive approximation data

- void increment_order ()

  increments polynomial expansion order (PCE, FT)

- void decrement_order ()

  decrements polynomial expansion order (PCE, FT)

Private Member Functions

- Pecos::SharedBasisApproxData & pecos_shared_data ()

  return pecosSharedData

- std::shared_ptr
  < Pecos::SharedPolyApproxData > pecos_shared_data_rep ()

  return pecosSharedDataRep

- void approx_type_to_basis_type (const String &approx_type, short &basis_type)

  utility to convert Dakota type string to Pecos type enumeration

Private Attributes

- Pecos::SharedBasisApproxData pecosSharedData

  the Pecos shared approximation data

- std::shared_ptr
  < Pecos::SharedPolyApproxData > pecosSharedDataRep

  convenience pointer to derived letter within pecosSharedData

Friends

- class **PecosApproximation**

Additional Inherited Members

14.249.1 Detailed Description

Derived approximation class for global basis polynomials.

The SharedPecosApproxData class provides a global approximation based on basis polynomials. This includes orthogonal polynomials used for polynomial chaos expansions and interpolation polynomials used for stochastic collocation.

14.249.2 Member Function Documentation

14.249.2.1 size_t push_index (const Pecos::ActiveKey & *key*) [inline], [protected], [virtual]

In Pecos, SharedPolyApproxData::push_index() is for internal use as it can be either a flattened (ISGDriver) or level-specific index (HSGDriver), as convenient for combined or hierarchical data restoration. SharedPolyApprox-Data::{restore,finalize}_index() are intended for external use and will map from push_index() to provide a consistent (flattened) representation. Dakota, however, does not make this distinction and uses {push,finalize}_index() semantics for consistency with {push,finalize}_data().

Reimplemented from SharedApproxData.

References SharedPecosApproxData::pecosSharedDataRep.

The documentation for this class was generated from the following files:

- SharedPecosApproxData.hpp
- SharedPecosApproxData.cpp

14.250 SharedResponseData Class Reference

Container class encapsulating variables data that can be shared among a set of Response instances.

Public Member Functions

- SharedResponseData ()

  default constructor
- SharedResponseData (const ProblemDescDB &problem_db)

  standard constructor
- SharedResponseData (const ActiveSet &set)

  alternate on-the-fly constructor (explicit disallows its use for implicit type conversion so that instantiations of Response(set) are invalid)
- SharedResponseData (const SharedResponseData &srd)

  copy constructor
- ∼SharedResponseData ()

  destructor
- SharedResponseData & operator= (const SharedResponseData &srd)

  assignment operator
- bool operator== (const SharedResponseData &other)

  experimental operator== for use in unit testing
- size_t num_scalar_responses () const

  number of scalar responses: primary_scalar + nonlinear constraints; note that these are non-contiguous when primary fields are present.
- size_t num_scalar_primary () const

  number of scalar primary responses (objectives, calibration terms, generic)
- size_t num_field_response_groups () const

  number of primary fields (primary field groups)
- size_t num_response_groups () const

  total number of response groups (number scalars + number pri field groups)
- size_t num_field_functions () const

  total number of primary field functions (elements); 1-norm of priFieldLengths
- size_t num_primary_functions () const

  number of primary functions (pri scalars + 1-norm of priFieldLengths)
- size_t num_functions () const

  total number of response functions (pri scalars + 1-norm of priFieldLengths + secondary scalars)
- const IntVector & field_lengths () const

  length of each primary field
- void field_lengths (const IntVector &field_lens)

  set field lengths (e.g., if experiment different from simulation)
- const IntVector & num_coords_per_field () const

  number of independent coordinates for each primary field
- const String & function_label (size_t i) const

  return a response function identifier string
- const StringArray & function_labels () const

  return the response function identifier strings
- StringArray & function_labels ()

return the response function identifier strings
- void function_label (const String &label, size_t i)

  set a response function identifier string
- void function_labels (const StringArray &labels)

  set the response function identifier strings
- const StringArray & field_group_labels () const

  return the coarse (per-group) primary field response labels
- void field_group_labels (const StringArray &field_labels)

  set the coarse primary field group labels (must agree with number fields)
- const String & responses_id () const

  return the response identifier
- short response_type () const

  return the response type: {BASE,SIMULATION,EXPERIMENT}_RESPONSE
- void response_type (short type)

  set the response type: {BASE,SIMULATION,EXPERIMENT}_RESPONSE
- short primary_fn_type () const

  get the primary function type (generic, objective, calibration)
- void primary_fn_type (short type)

  set the primary function type (generic, objective, calibration)
- const RealVector & simulation_error () const

  retrieve simulation variance
- const StringArray & metadata_labels () const

  get labels for metadata fields
- void metadata_labels (const StringArray &md_labels)

  set labels for metadata fields
- void read_annotated (std::istream &s, size_t num_md)

  read metadata labels from annotated (neutral) file
- SharedResponseData copy () const

  create a deep copy of the current object and return by value
- void reshape (size_t num_fns)

  reshape the data, disconnecting a shared rep if necessary
- void reshape_metadata (size_t num_meta)

  reshape the shared metadata (labels only at this time)
- void reshape_labels (StringArray &resp_labels, size_t num_fns)

  reshape the response labels using inflation/deflation if possible
- bool is_null () const

  return true if empty handle with null representation
- long reference_count () const

  how many handles (including this) are sharing this representation (body); for debugging/testing only
- template<class Archive >
  void **serialize** (Archive &ar, const unsigned int version)

Private Member Functions

- template<class Archive >
  void serialize (Archive &ar, const unsigned int version)

  serialize through the pointer, which requires object tracking: write and read are symmetric for this class

Private Attributes

- boost::shared_ptr
  < SharedResponseDataRep > srdRep

  pointer to the body (handle-body idiom)

Friends

- class boost::serialization::access

  allow boost access to serialize this class

14.250.1 Detailed Description

Container class encapsulating variables data that can be shared among a set of Response instances.

An array of Response objects (e.g., Analyzer::allResponse) contains repeated configuration data (id's, labels, counts). SharedResponseData employs a handle-body idiom to allow this shared data to be managed in a single object with many references to it, one per Response object in the array. This allows scaling to larger sample sets.

14.250.2 Member Function Documentation

14.250.2.1 SharedResponseData copy ( ) const

create a deep copy of the current object and return by value

Deep copies are used when recasting changes the nature of a Response set.

References SharedResponseData::srdRep.

Referenced by ExperimentData::add_data(), ExperimentData::ExperimentData(), ExperimentData::initialize(), and ExperimentData::load_data().

The documentation for this class was generated from the following files:

- SharedResponseData.hpp
- SharedResponseData.cpp

14.251 SharedResponseDataRep Class Reference

The representation of a SharedResponseData instance. This representation, or body, may be shared by multiple SharedResponseData handle instances.

Public Member Functions

- ∼SharedResponseDataRep ()

  destructor must be public for shared_ptr

- template<class Archive >
  void **serialize** (Archive &ar, const unsigned int version)

Private Member Functions

- SharedResponseDataRep ()

  default constructor

- SharedResponseDataRep (const ProblemDescDB &problem_db)

  standard constructor
- SharedResponseDataRep (const ActiveSet &set)

  alternate on-the-fly constructor
- void copy_rep (SharedResponseDataRep ∗srd_rep)

  copy the data from srd_rep to the current representation
- template<class Archive >
  void serialize (Archive &ar, const unsigned int version)

  serialize the core shared response data: write and read are symmetric for this class
- bool operator== (const SharedResponseDataRep &other)

  experimental operator== for use in unit testing
- void build_field_labels (const StringArray &labels_per_group)

  populate functionLabels with scalar and unrolled field labels based on fieldLabels and group lengths
- void **resize_field_labels** (const StringArray &old_full_labels, size_t old_field_elements)
- void update_field_labels ()

  update functionLabels with unrolled field labels based on fieldLabels and group lengths
- std::string primary_fn_name () const

  the primary function type as a friendly string, e.g., "objective_functions"

Private Attributes

- short responseType

  enumeration of BASE_RESPONSE, SIMULATION_RESPONSE, or EXPERIMENT_RESPONSE
- short primaryFnType

  data set type for primary response: generic, objective, calibration
- String responsesId

  response identifier string from the input file
- StringArray functionLabels

  fine-grained (unrolled) set of response function identifiers used to improve output readability; length Response::functionValues
- StringArray priFieldLabels

  labels for each primary response field
- RealVector simulationVariance

  simulation variance
- size_t numScalarResponses = 0

  number of scalar responses (scalar primary + scalar constraints)
- size_t numScalarPrimary = 0

  number of scalar primary reponses (secondary computed from difference)
- IntVector priFieldLengths

  length of each primary response field
- IntVector coordsPerPriField

  number of independent coordinates, e.g., x, t, for each field f(x,t)
- StringArray metadataLabels

  descriptors for metadata fields (empty if none)

Friends

- class **SharedResponseData**
- class boost::serialization::access

  allow boost access to serialize this class

14.251.1 Detailed Description

The representation of a SharedResponseData instance. This representation, or body, may be shared by multiple SharedResponseData handle instances.

The SharedResponseData/SharedResponseDataRep pairs utilize a handle-body idiom (Coplien, Advanced C++).

14.251.2 Member Function Documentation

14.251.2.1 void copy_rep (SharedResponseDataRep * *srd_rep*) [private]

copy the data from srd_rep to the current representation

Deep copies are used when recasting changes the nature of a Response set.

References SharedResponseDataRep::coordsPerPriField, SharedResponseDataRep::functionLabels, SharedResponseDataRep::metadataLabels, SharedResponseDataRep::numScalarPrimary, SharedResponseDataRep::numScalarResponses, SharedResponseDataRep::priFieldLabels, SharedResponseDataRep::priFieldLengths, SharedResponseDataRep::primaryFnType, SharedResponseDataRep::responsesId, SharedResponseDataRep::responseType, and SharedResponseDataRep::simulationVariance.

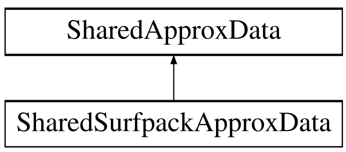
The documentation for this class was generated from the following files:

- SharedResponseData.hpp
- SharedResponseData.cpp

14.252 SharedSurfpackApproxData Class Reference

Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.

Inheritance diagram for SharedSurfpackApproxData:



Public Member Functions

- SharedSurfpackApproxData ()

  default constructor
- SharedSurfpackApproxData (const String &approx_type, const UShortArray &approx_order, size_t num_vars, short data_order, short output_level)

  alternate constructor
- SharedSurfpackApproxData (ProblemDescDB &problem_db, size_t num_vars)

  standard constructor: Surfpack surface of appropriate type will be created
- ∼SharedSurfpackApproxData ()

  destructor

Private Member Functions

- void add_sd_to_surfdata (const Pecos::SurrogateDataVars &sdv, const Pecos::SurrogateDataResp &sdr, short fail_code, SurfData &surf_data)

add Pecos::SurrogateData::SurrogateData{Vars,Resp} to SurfData, accounting for buildDataOrder available

- void copy_matrix (const RealSymMatrix &rsm, SurfpackMatrix< Real > &surfpack_matrix)

  copy RealSymMatrix to SurfpackMatrix (Real type only)
- template<typename RealArrayType >
  void merge_variable_arrays (const RealVector &cv, const IntVector &div, const RealVector &drv, RealArrayType &ra)

  merge cv, div, and drv vectors into a single ra array
- template<typename RealArrayType >
  void sdv_to_realarray (const Pecos::SurrogateDataVars &sdv, RealArrayType &ra)

  aggregate {continuous,discrete int,discrete real} variables from SurrogateDataVars into ra
- template<typename RealArrayType >
  void vars_to_realarray (const Variables &vars, RealArrayType &ra)

  aggregate {active,all} {continuous,discrete int,discrete real} variables into pre-sized array
- template<typename RealArrayType >
  void active_vars_to_realarray (const Variables &vars, RealArrayType &ra)

  aggregate active {continuous,discrete int,discrete real} variables into pre-sized array
- template<typename RealArrayType >
  void all_vars_to_realarray (const Variables &vars, RealArrayType &ra)

  aggregate all {continuous,discrete int,discrete real} variables into pre-sized array
- StringArray variable_labels (const Variables &vars) const

  retrieve the active or all labels over which the surrogate was built
- void validate_metrics (const std::set< std::string > &allowed_metrics)

  validate metric names and cross validation options
- unsigned compute_folds ()

  compute number of folds from numFols/percentFold
- void map_variable_labels (const Variables &dfsm_vars, const StringArray &approx_labels)

  validate imported labels and initialize map if needed
- template<typename RealArrayType >
  RealArrayType imported_eval_vars (const Variables &vars)

  when importing, take all view of vars and permute as needed

Private Attributes

- std::vector< size_t > varsMapIndices

  If populated, reorder variables when evaluating surrogate these are indices into the Model's vars so approx_eval[i] = [model_vars[ind[i]]].
- unsigned short approxOrder

  order of polynomial approximation
- StringArray diagnosticSet

  set of diagnostic metrics
- bool crossValidateFlag

  whether to perform cross validation
- unsigned numFolds

  number of folds for CV
- Real percentFold

  percentage of data for CV
- bool pressFlag

  whether to perform PRESS

Friends

- class **SurfpackApproximation**
- class **VPSApproximation**
- class **SurrogatesBaseApprox**
- class **SurrogatesGPApprox**
- class **SurrogatesPolyApprox**

Additional Inherited Members

14.252.1 Detailed Description

Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.

The SharedSurfpackApproxData class is the interface between Dakota and Surfpack. Based on the information in the ProblemDescDB that is passed in through the constructor, SharedSurfpackApproxData builds a Surfpack Surface object that corresponds to one of the following data-fitting techniques: polynomial regression, kriging, artificial neural networks, radial basis function network, or multivariate adaptaive regression splines (MARS).

14.252.2 Constructor & Destructor Documentation

14.252.2.1 SharedSurfpackApproxData (const String & *approx_type,* const UShortArray & *approx_order,* size_t *num_vars,* short *data_order,* short *output_level*)

alternate constructor

On-the-fly constructor which uses mostly Surfpack model defaults.

References Dakota::abort_handler(), SharedSurfpackApproxData::approxOrder, and SharedApproxData::approxType.

14.252.2.2 SharedSurfpackApproxData (ProblemDescDB & *problem_db,* size_t *num_vars*)

standard constructor: Surfpack surface of appropriate type will be created

Initialize the embedded Surfpack surface object and configure it using the specifications from the input file. Data for the surface is created later.

References SharedSurfpackApproxData::approxOrder, SharedApproxData::approxType, ProblemDescDB::get_short(), and ProblemDescDB::get_string().

The documentation for this class was generated from the following files:

- SharedSurfpackApproxData.hpp
- SharedSurfpackApproxData.cpp

14.253 SharedVariablesData Class Reference

Container class encapsulating variables data that can be shared among a set of Variables instances.

Public Member Functions

- SharedVariablesData ()

  default constructor
- SharedVariablesData (const ProblemDescDB &problem_db, const std::pair$<$ short, short $>$ &view)

standard constructor

- SharedVariablesData (const std::pair< short, short > &view, const std::map< unsigned short, size_t > &vars_comps, const BitArray &all_relax_di=BitArray(), const BitArray &all_relax_dr=BitArray())

    medium weight constructor providing detailed variable counts
- SharedVariablesData (const std::pair< short, short > &view, const SizetArray &vars_comps_totals, const BitArray &all_relax_di=BitArray(), const BitArray &all_relax_dr=BitArray())

    lightweight constructor providing variable count totals
- SharedVariablesData (const SharedVariablesData &svd)

    copy constructor
- ~SharedVariablesData ()

    destructor
- SharedVariablesData & operator= (const SharedVariablesData &svd)

    assignment operator
- SharedVariablesData copy () const

    create a deep copy of the current object and return by value
- void all_counts (size_t &num_acv, size_t &num_adiv, size_t &num_adsv, size_t &num_adrv) const

    compute all variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete{Int,Real}
- void design_counts (size_t &num_cdv, size_t &num_ddiv, size_t &num_ddsv, size_t &num_ddrv) const

    compute design variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete{Int,Real}
- void aleatory_uncertain_counts (size_t &num_cauv, size_t &num_dauiv, size_t &num_dausv, size_t &num_daurv) const

    compute aleatory uncertain variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete{Int,Real}
- void epistemic_uncertain_counts (size_t &num_ceuv, size_t &num_deuiv, size_t &num_deusv, size_t &num_deurv) const

    compute epistemic uncertain variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete{Int,Real}
- void uncertain_counts (size_t &num_cuv, size_t &num_duiv, size_t &num_dusv, size_t &num_durv) const

    compute uncertain variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete{Int,Real}
- void state_counts (size_t &num_csv, size_t &num_dsiv, size_t &num_dssv, size_t &num_dsrv) const

    compute state variables sums from SharedVariablesDataRep::variablesCompsTotals and SharedVariablesDataRep::allRelaxedDiscrete{Int,Real}
- void active_subsets (bool &cdv, bool &ddv, bool &cauv, bool &dauv, bool &ceuv, bool &deuv, bool &csv, bool &dsv) const

    define active variable subsets based on active view
- void inactive_subsets (bool &cdv, bool &ddv, bool &cauv, bool &dauv, bool &ceuv, bool &deuv, bool &csv, bool &dsv) const

    define active variable subsets based on active view
- void complement_subsets (bool &cdv, bool &ddv, bool &cauv, bool &dauv, bool &ceuv, bool &deuv, bool &csv, bool &dsv) const

    define active variable subsets based on active view
- size_t cv_index_to_all_index (size_t cv_index) const

    convert index within active continuous variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t icv_index_to_all_index (size_t ccv_index) const

    convert index within inactive continuous variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t ccv_index_to_all_index (size_t ccv_index) const

    convert index within complement of active continuous variables to index within aggregated variables (all continous, discrete {int,string,real})

- size_t acv_index_to_all_index (size_t acv_index) const

    convert index within all continuous variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t div_index_to_all_index (size_t div_index) const

    convert index within active discrete integer variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t idiv_index_to_all_index (size_t div_index) const

    convert index within inactive discrete integer variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t cdiv_index_to_all_index (size_t div_index) const

    convert index within complement of active discrete integer variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t adiv_index_to_all_index (size_t adiv_index) const

    convert index within all discrete integer variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t dsv_index_to_all_index (size_t dsv_index) const

    convert index within active discrete string variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t idsv_index_to_all_index (size_t dsv_index) const

    convert index within inactive discrete string variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t cdsv_index_to_all_index (size_t dsv_index) const

    convert index within complement of active discrete string variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t adsv_index_to_all_index (size_t adsv_index) const

    convert index within all discrete string variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t drv_index_to_all_index (size_t drv_index) const

    convert index within active discrete real variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t idrv_index_to_all_index (size_t drv_index) const

    convert index within inactive discrete real variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t cdrv_index_to_all_index (size_t drv_index) const

    convert index within complement of active discrete real variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t adrv_index_to_all_index (size_t adrv_index) const

    convert index within all discrete real variables to index within aggregated variables (all continous, discrete {int,string,real})
- size_t cv_index_to_active_index (size_t cv_index) const

    convert index within active continuous variables to index within aggregated active variables (active continous, discrete {int,string,real})
- size_t div_index_to_active_index (size_t div_index) const

    convert index within active discrete integer variables to index within aggregated active variables (active continous, discrete {int,string,real})
- size_t dsv_index_to_active_index (size_t dsv_index) const

    convert index within active discrete string variables to index within aggregated active variables (active continous, discrete {int,string,real})
- size_t drv_index_to_active_index (size_t drv_index) const

    convert index within active discrete real variables to index within aggregated active variables (active continous, discrete {int,string,real})
- size_t ccv_index_to_acv_index (size_t ccv_index) const

    convert index within complement of active continuous variables to index within all continuous variables
- size_t cdiv_index_to_adiv_index (size_t div_index) const

convert index within complement of active discrete integer variables to index within all discrete integer variables

- size_t cdsv_index_to_adsv_index (size_t dsv_index) const

  convert index within complement of active discrete string variables to index within all discrete string variables
- size_t cdrv_index_to_adrv_index (size_t drv_index) const

  convert index within complement of active discrete real variables to index within all discrete real variables
- BitArray cv_to_all_mask () const

  create a BitArray indicating the active continuous subset of all {continuous,discrete {int,string,real}} variables
- BitArray icv_to_all_mask () const

  create a BitArray indicating the inactive continuous subset of all {continuous,discrete {int,string,real}} variables
- BitArray ccv_to_all_mask () const

  create a BitArray indicating the complement continuous subset of all {continuous,discrete {int,string,real}} variables
- BitArray acv_to_all_mask () const

  create a BitArray indicating the all continuous subset of all {continuous,discrete {int,string,real}} variables
- BitArray div_to_all_mask () const

  create a BitArray indicating the active discrete int subset of all {continuous,discrete {int,string,real}} variables
- BitArray idiv_to_all_mask () const

  create a BitArray indicating the inactive discrete int subset of all {continuous,discrete {int,string,real}} variables
- BitArray cdiv_to_all_mask () const

  create a BitArray indicating the complement discrete int subset of all {continuous,discrete {int,string,real}} variables
- BitArray adiv_to_all_mask () const

  create a BitArray indicating the all discrete int subset of all {continuous,discrete {int,string,real}} variables
- BitArray dsv_to_all_mask () const

  create a BitArray indicating the active discrete string subset of all {continuous,discrete {int,string,real}} variables
- BitArray idsv_to_all_mask () const

  create a BitArray indicating the inactive discrete string subset of all {continuous,discrete {int,string,real}} variables
- BitArray cdsv_to_all_mask () const

  create a BitArray indicating the complement discrete string subset of all {continuous,discrete {int,string,real}} variables
- BitArray adsv_to_all_mask () const

  create a BitArray indicating the all discrete string subset of all {continuous,discrete {int,string,real}} variables
- BitArray drv_to_all_mask () const

  create a BitArray indicating the active discrete real subset of all {continuous,discrete {int,string,real}} variables
- BitArray idrv_to_all_mask () const

  create a BitArray indicating the inactive discrete real subset of all {continuous,discrete {int,string,real}} variables
- BitArray cdrv_to_all_mask () const

  create a BitArray indicating the complement discrete real subset of all {continuous,discrete {int,string,real}} variables
- BitArray adrv_to_all_mask () const

  create a BitArray indicating the all discrete real subset of all {continuous,discrete {int,string,real}} variables
- void initialize_active_start_counts ()

  initialize start index and counts for active variables
- void initialize_inactive_start_counts ()

  initialize start index and counts for inactive variables
- void initialize_active_components ()

  initialize the active components totals given active variable counts
- void initialize_inactive_components ()

  initialize the inactive components totals given inactive variable counts
- const BitArray & all_relaxed_discrete_int () const

  return allRelaxedDiscreteInt
- const BitArray & all_relaxed_discrete_real () const

  return allRelaxedDiscreteReal
- StringMultiArrayView all_continuous_labels (size_t start, size_t num_items) const

  get num_items continuous labels beginning at index start

- void all_continuous_labels (StringMultiArrayConstView cv_labels, size_t start, size_t num_items)
  set num_items continuous labels beginning at index start
- void all_continuous_label (const String &cv_label, size_t index)
  set continuous label at index start
- StringMultiArrayView all_discrete_int_labels (size_t start, size_t num_items) const
  get num_items discrete integer labels beginning at index start
- void all_discrete_int_labels (StringMultiArrayConstView div_labels, size_t start, size_t num_items)
  set num_items discrete integer labels beginning at index start
- void all_discrete_int_label (const String &div_label, size_t index)
  set discrete integer label at index start
- StringMultiArrayView all_discrete_string_labels (size_t start, size_t num_items) const
  get num_items discrete string labels beginning at index start
- void all_discrete_string_labels (StringMultiArrayConstView dsv_labels, size_t start, size_t num_items)
  set num_items discrete string labels beginning at index start
- void all_discrete_string_label (const String &dsv_label, size_t index)
  set discrete string label at index start
- StringMultiArrayView all_discrete_real_labels (size_t start, size_t num_items) const
  get num_items discrete real labels beginning at index start
- void all_discrete_real_labels (StringMultiArrayConstView drv_labels, size_t start, size_t num_items)
  set num_items discrete real labels beginning at index start
- void all_discrete_real_label (const String &drv_label, size_t index)
  set discrete real label at index start
- void assemble_all_labels (StringArray &all_labels) const
  assemble all variable labels (continuous and discrete {int,string,real}) in standard (input specification-based) order
- UShortMultiArrayConstView all_continuous_types (size_t start, size_t num_items) const
  get num_items continuous types beginning at index start
- void all_continuous_types (UShortMultiArrayConstView cv_types, size_t start, size_t num_items)
  set num_items continuous types beginning at index start
- void all_continuous_type (unsigned short cv_type, size_t index)
  set continuous type at index
- UShortMultiArrayConstView all_discrete_int_types (size_t start, size_t num_items) const
  get num_items discrete integer types beginning at index start
- void all_discrete_int_types (UShortMultiArrayConstView div_types, size_t start, size_t num_items)
  set num_items discrete integer types beginning at index start
- void all_discrete_int_type (unsigned short div_type, size_t index)
  set discrete integer type at index
- UShortMultiArrayConstView all_discrete_string_types (size_t start, size_t num_items) const
  get num_items discrete string types beginning at index start
- void all_discrete_string_types (UShortMultiArrayConstView dsv_types, size_t start, size_t num_items)
  set num_items discrete string types beginning at index start
- void all_discrete_string_type (unsigned short dsv_type, size_t index)
  set discrete string type at index
- UShortMultiArrayConstView all_discrete_real_types (size_t start, size_t num_items) const
  get num_items discrete real types beginning at index start
- void all_discrete_real_types (UShortMultiArrayConstView drv_types, size_t start, size_t num_items)
  set num_items discrete real types beginning at index start
- void all_discrete_real_type (unsigned short drv_type, size_t index)
  set discrete real type at index
- SizetMultiArrayConstView all_continuous_ids (size_t start, size_t num_items) const
  get num_items continuous ids beginning at index start
- void all_continuous_ids (SizetMultiArrayConstView cv_ids, size_t start, size_t num_items)

set num_items continuous ids beginning at index start

- void all_continuous_id (size_t id, size_t index)

  set num_items continuous ids beginning at index start

- SizetMultiArrayConstView all_discrete_int_ids (size_t start, size_t num_items) const

  get num_items discrete int ids beginning at index start

- SizetMultiArrayConstView all_discrete_string_ids (size_t start, size_t num_items) const

  get num_items discrete string ids beginning at index start

- SizetMultiArrayConstView all_discrete_real_ids (size_t start, size_t num_items) const

  get num_items discrete real ids beginning at index start

- const String & id () const

  return the user-provided or default Variables identifier

- const SizetArray & components_totals () const

  return variable type counts for {continuous,discrete integer,discrete real} {design,aleatory uncertain,epistemic uncertain,state}

- const SizetArray & active_components_totals () const

  return active variable type counts for {continuous,discrete integer,discrete real} {design,aleatory uncertain,epistemic uncertain,state}

- const SizetArray & inactive_components_totals () const

  return inactive variable type counts for {continuous,discrete integer,discrete real} {design,aleatory uncertain,epistemic uncertain,state}

- size_t vc_lookup (unsigned short key) const

  retrieve the variables type count within svdRep->variablesComponents corresponding to (a fine-grain variables type) key

- const std::pair< short, short > & view () const

  retreive the Variables view

- void inactive_view (short view2)

  set the inactive Variables view

- size_t cv () const

  get number of active continuous vars

- size_t cv_start () const

  get start index of active continuous vars

- size_t div () const

  get number of active discrete int vars

- size_t div_start () const

  get start index of active discrete int vars

- size_t dsv () const

  get number of active discrete string vars

- size_t dsv_start () const

  get start index of active discrete string vars

- size_t drv () const

  get number of active discrete real vars

- size_t drv_start () const

  get start index of active discrete real vars

- size_t icv () const

  get number of inactive continuous vars

- size_t icv_start () const

  get start index of inactive continuous vars

- size_t idiv () const

  get number of inactive discrete int vars

- size_t idiv_start () const

  get start index of inactive discrete int vars

- size_t idsv () const

  get number of inactive discrete string vars
- size_t idsv_start () const

  get start index of inactive discr string vars
- size_t idrv () const

  get number of inactive discrete real vars
- size_t idrv_start () const

  get start index of inactive discrete real vars
- void cv (size_t ncv)

  set number of active continuous vars
- void cv_start (size_t cvs)

  set start index of active continuous vars
- void div (size_t ndiv)

  set number of active discrete int vars
- void div_start (size_t divs)

  set start index of active discrete int vars
- void dsv (size_t ndsv)

  set number of active discrete string vars
- void dsv_start (size_t dsvs)

  set start index of active discr string vars
- void drv (size_t ndrv)

  set number of active discrete real vars
- void drv_start (size_t drvs)

  set start index of active discrete real vars
- void icv (size_t nicv)

  set number of inactive continuous vars
- void icv_start (size_t icvs)

  set start index of inactive continuous vars
- void idiv (size_t nidiv)

  set number of inactive discrete int vars
- void idiv_start (size_t idivs)

  set start index of inactive discr int vars
- void idsv (size_t nidsv)

  set number of inactive discr string vars
- void idsv_start (size_t idsvs)

  set start index of inact discr string vars
- void idrv (size_t nidrv)

  set number of inactive discrete real vars
- void idrv_start (size_t idrvs)

  set start index of inact discr real vars
- template<class Archive >
  void **serialize** (Archive &ar, const unsigned int version)

Private Member Functions

- template<class Archive >
  void serialize (Archive &ar, const unsigned int version)

  serialize through the pointer, which requires object tracking: write and read are symmetric for this class

Private Attributes

- boost::shared_ptr
  < SharedVariablesDataRep > svdRep

  pointer to the body (handle-body idiom)

Friends

- class boost::serialization::access

  allow boost access to serialize this class

14.253.1 Detailed Description

Container class encapsulating variables data that can be shared among a set of Variables instances.

An array of Variables objects (e.g., Analyzer::allVariables) contains repeated configuration data (id's, labels, counts). SharedVariablesData employs a handle-body idiom to allow this shared data to be managed in a single object with many references to it, one per Variables object in the array. This allows scaling to larger sample sets.

14.253.2 Member Function Documentation

14.253.2.1 SharedVariablesData copy ( ) const

create a deep copy of the current object and return by value

Deep copies are used when recasting changes the nature of a Variables set.

References Dakota::svd(), and SharedVariablesData::svdRep.

Referenced by ExperimentData::add_data(), NonDBayesCalibration::add_lhs_hifi_data(), ExperimentData::-ExperimentData(), ExperimentData::load_data(), and Model::Model().

The documentation for this class was generated from the following files:

- SharedVariablesData.hpp
- SharedVariablesData.cpp

14.254 SharedVariablesDataRep Class Reference

The representation of a SharedVariablesData instance. This representation, or body, may be shared by multiple SharedVariablesData handle instances.

Public Member Functions

- ∼SharedVariablesDataRep ()

  destructor must be public for shared_ptr

- template<class Archive >
  void **save** (Archive &ar, const unsigned int version) const
- template<class Archive >
  void **load** (Archive &ar, const unsigned int version)

Private Member Functions

- SharedVariablesDataRep (const ProblemDescDB &problem_db, const std::pair< short, short > &view)

  standard constructor
- SharedVariablesDataRep (const std::pair< short, short > &view, const std::map< unsigned short, size_t > &vars_comps, const BitArray &all_relax_di, const BitArray &all_relax_dr)

  medium weight constructor providing detailed variable counts
- SharedVariablesDataRep (const std::pair< short, short > &view, const SizetArray &vars_comps_totals, const BitArray &all_relax_di, const BitArray &all_relax_dr)

  lightweight constructor providing variable count totals
- SharedVariablesDataRep ()

  default constructor
- void initialize_components_totals (const ProblemDescDB &problem_db)

  populate variables{Components,CompsTotals} from user variable type and count specifications
- void components_to_totals ()

  update variablesCompsTotals from variablesComponents
- void relax_noncategorical (const ProblemDescDB &problem_db)

  populate allRelaxedDiscrete{Int,Real} from user specifications (relax variables that are not declared as categorical)
- void set_relax (const BitArray &user_cat_spec, size_t ucs_index, size_t ard_cntr, BitArray &ard_container)

  Set the ard_cntr entry in the all-relaxed-discrete integer or real container ard_container, based on user-specification of categorical, accounting for empty.
- void all_counts (size_t &num_acv, size_t &num_adiv, size_t &num_adsv, size_t &num_adrv) const

  compute all variables sums from variablesCompsTotals
- void relax_counts (size_t &num_cv, size_t &num_div, size_t &num_drv, size_t offset_di, size_t offset_dr) const

  adjust counts based on allRelaxedDiscrete{Int,Real}
- void design_counts (size_t &num_cdv, size_t &num_ddiv, size_t &num_ddsv, size_t &num_ddrv) const

  compute design variables sums from variablesCompsTotals
- void aleatory_uncertain_counts (size_t &num_cauv, size_t &num_dauiv, size_t &num_dausv, size_t &num_-daurv) const

  compute aleatory uncertain variables sums from variablesCompsTotals
- void epistemic_uncertain_counts (size_t &num_ceuv, size_t &num_deuiv, size_t &num_deusv, size_t &num-_deurv) const

  compute epistemic uncertain variables sums from variablesCompsTotals
- void uncertain_counts (size_t &num_cuv, size_t &num_duiv, size_t &num_dusv, size_t &num_durv) const

  compute uncertain variables sums from variablesCompsTotals
- void state_counts (size_t &num_csv, size_t &num_dsiv, size_t &num_dssv, size_t &num_dsrv) const

  compute state variables sums from variablesCompsTotals
- void view_start_counts (short view, size_t &cv_start, size_t &div_start, size_t &dsv_start, size_t &drv_start, size_t &num_cv, size_t &num_div, size_t &num_dsv, size_t &num_drv) const

  define start indices and counts for active variables based on view
- void view_subsets (short view, bool &cdv, bool &ddv, bool &cauv, bool &dauv, bool &ceuv, bool &deuv, bool &csv, bool &dsv) const

  define active variable subsets based on active view
- void size_all_labels ()

  size all{Continuous,DiscreteInt,DiscreteString,DiscreteReal}Labels, with or without discrete relaxation
- void size_all_types ()

  size all{Continuous,DiscreteInt,DiscreteString,DiscreteReal}Types, with or without discrete relaxation
- size_t cv_index_to_all_index (size_t cv_index, bool cdv, bool cauv, bool ceuv, bool csv) const

  convert index within active continuous variables (as identified by bools) to index within aggregated variables (all continous, discrete {int,string,real})
- size_t div_index_to_all_index (size_t div_index, bool ddv, bool dauv, bool deuv, bool dsv) const

convert index within active discrete integer variables (as identified by bools) to index within aggregated variables (all continous, discrete {int,string,real})

- size_t dsv_index_to_all_index (size_t dsv_index, bool ddv, bool dauv, bool deuv, bool dsv) const

  convert index within active discrete string variables (as identified by bools) to index within aggregated variables (all continous, discrete {int,string,real})
- size_t drv_index_to_all_index (size_t drv_index, bool ddv, bool dauv, bool deuv, bool dsv) const

  convert index within active discrete real variables (as identified by bools) to index within aggregated variables (all continous, discrete {int,string,real})
- BitArray cv_to_all_mask (bool cdv, bool cauv, bool ceuv, bool csv) const

  create a BitArray indicating the active continuous subset of all {continuous,discrete {int,string,real}} variables
- BitArray div_to_all_mask (bool ddv, bool dauv, bool deuv, bool dsv) const

  create a BitArray indicating the active discrete int subset of all {continuous,discrete {int,string,real}} variables
- BitArray dsv_to_all_mask (bool ddv, bool dauv, bool deuv, bool dsv) const

  create a BitArray indicating the active discrete string subset of all {continuous,discrete {int,string,real}} variables
- BitArray drv_to_all_mask (bool ddv, bool dauv, bool deuv, bool dsv) const

  create a BitArray indicating the active discrete real subset of all {continuous,discrete {int,string,real}} variables
- void initialize_all_labels (const ProblemDescDB &problem_db)

  aggregate all{Continuous,DiscreteInt,DiscreteString,DiscreteReal}Labels from user specification or defaults
- void initialize_all_types ()

  initialize all{Continuous,DiscreteInt,DiscreteString,DiscreteReal}Types, with or without discrete relaxation
- void initialize_all_ids ()

  initialize allContinuousIds (discrete not currently needed), with or without discrete relaxation
- void initialize_active_start_counts ()

  initialize {c,di,ds,dr}vStart and num{D,DI,DS,DR}V
- void initialize_inactive_start_counts ()

  initialize i{c,di,ds,dr}vStart and numI{D,DI,DS,DR}V
- void initialize_active_components ()

  initialize activeVarsCompsTotals given {c,di,dr}vStart and num{C,DI,DR}V
- void initialize_inactive_components ()

  initialize inactiveVarsCompsTotals given i{c,di,dr}vStart and numI{C,DI,DR}V
- size_t vc_lookup (unsigned short key) const

  retrieve the count within variablesComponents corresponding to key
- void copy_rep (SharedVariablesDataRep ∗svd_rep)

  copy the data from svd_rep to the current representation
- template<class Archive >
  void save (Archive &ar, const unsigned int version) const

  serialize the core shared variables data
- template<class Archive >
  void load (Archive &ar, const unsigned int version)

  load the core shared variables data and restore class state
- BOOST_SERIALIZATION_SPLIT_MEMBER () String variablesId

  variables identifier string from the input file

Private Attributes

- std::map< unsigned short, size_t > variablesComponents

  map linking variable types to counts
- SizetArray variablesCompsTotals

  totals for variable type counts for {continuous,discrete integer,discrete string,discrete real} {design,aleatory uncertain,epistemic uncertain,state}.
- SizetArray activeVarsCompsTotals

totals for active variable type counts for {continuous,discrete integer,discrete string,discrete real} {design,aleatory uncertain,epistemic uncertain,state}.

- SizetArray inactiveVarsCompsTotals

  totals for inactive variable type counts for {continuous,discrete integer,discrete string,discrete real} {design,aleatory uncertain,epistemic uncertain,state}.

- std::pair< short, short > variablesView

  the variables view pair containing active (first) and inactive (second) view enumerations

- size_t cvStart

  start index of active continuous variables within allContinuousVars

- size_t divStart

  start index of active discrete integer variables within allDiscreteIntVars

- size_t dsvStart

  start index of active discrete string vars within allDiscreteStringVars

- size_t drvStart

  start index of active discrete real variables within allDiscreteRealVars

- size_t icvStart

  start index of inactive continuous variables within allContinuousVars

- size_t idivStart

  start index of inactive discrete integer vars within allDiscreteIntVars

- size_t idsvStart

  start index of inactive discrete string vars within allDiscreteStringVars

- size_t idrvStart

  start index of inactive discrete real variables within allDiscreteRealVars

- size_t numCV

  number of active continuous variables

- size_t numDIV

  number of active discrete integer variables

- size_t numDSV

  number of active discrete string variables

- size_t numDRV

  number of active discrete real variables

- size_t numICV

  number of inactive continuous variables

- size_t numIDIV

  number of inactive discrete integer variables

- size_t numIDSV

  number of inactive discrete string variables

- size_t numIDRV

  number of inactive discrete real variables

- StringMultiArray allContinuousLabels

  array of variable labels for all of the continuous variables

- StringMultiArray allDiscreteIntLabels

  array of variable labels for all of the discrete integer variables

- StringMultiArray allDiscreteStringLabels

  array of variable labels for all of the discrete string variables

- StringMultiArray allDiscreteRealLabels

  array of variable labels for all of the discrete real variables

- UShortMultiArray allContinuousTypes

  array of variable types for all of the continuous variables

- UShortMultiArray allDiscreteIntTypes

  array of variable types for all of the discrete integer variables

- UShortMultiArray allDiscreteStringTypes

  array of variable types for all of the discrete string variables
- UShortMultiArray allDiscreteRealTypes

  array of variable types for all of the discrete real variables
- SizetMultiArray allContinuousIds

  array of 1-based position identifiers for the all continuous variables array
- SizetMultiArray allDiscreteIntIds

  array of 1-based ids (into total variable set) for discrete int
- SizetMultiArray allDiscreteStringIds

  array of 1-based ids (into total variable set) for discrete string
- SizetMultiArray allDiscreteRealIds

  array of 1-based ids (into total variable set) for discrete real
- BitArray allRelaxedDiscreteInt

  array of booleans to indicate relaxation (promotion from DiscreteInt to Continuous) for all specified discrete int variables Note: container will be empty when not relaxing variables
- BitArray allRelaxedDiscreteReal

  array of booleans to indicate relaxation (promotion from DiscreteReal to Continuous) for all specified discrete real variables Note: container will be empty when not relaxing variables

Friends

- class **SharedVariablesData**
- class boost::serialization::access

  allow boost access to serialize this class

14.254.1 Detailed Description

The representation of a SharedVariablesData instance. This representation, or body, may be shared by multiple SharedVariablesData handle instances.

The SharedVariablesData/SharedVariablesDataRep pairs utilize a handle-body idiom (Coplien, Advanced C++).

14.254.2 Member Function Documentation

14.254.2.1 void copy_rep (**SharedVariablesDataRep** * *svd_rep*) [private]

copy the data from svd_rep to the current representation

Deep copies are used when recasting changes the nature of a Variables set.

References SharedVariablesDataRep::activeVarsCompsTotals, SharedVariablesDataRep::allContinuousIds, SharedVariablesDataRep::allContinuousLabels, SharedVariablesDataRep::allContinuousTypes, SharedVariablesDataRep::allDiscreteIntIds, SharedVariablesDataRep::allDiscreteIntLabels, SharedVariablesDataRep::allDiscreteIntTypes, SharedVariablesDataRep::allDiscreteRealIds, SharedVariablesDataRep::allDiscreteRealLabels, SharedVariablesDataRep::allDiscreteRealTypes, SharedVariablesDataRep::allDiscreteStringIds, SharedVariablesDataRep::allDiscreteStringLabels, SharedVariablesDataRep::allDiscreteStringTypes, SharedVariablesDataRep::allRelaxedDiscreteInt, SharedVariablesDataRep::allRelaxedDiscreteReal, SharedVariablesDataRep::cvStart, SharedVariablesDataRep::divStart, SharedVariablesDataRep::drvStart, SharedVariablesDataRep::dsvStart, SharedVariablesDataRep::icvStart, SharedVariablesDataRep::idivStart, SharedVariablesDataRep::idrvStart, SharedVariablesDataRep::idsvStart, SharedVariablesDataRep::inactiveVarsCompsTotals, SharedVariablesDataRep::numCV, SharedVariablesDataRep::numDIV, SharedVariablesDataRep::numDRV, SharedVariablesDataRep::numDSV, SharedVariablesDataRep::numICV, SharedVariablesDataRep::numIDIV, SharedVariablesDataRep::numIDRV, SharedVariablesDataRep::numIDSV, SharedVariablesDataRep::variablesComponents, SharedVariablesDataRep::variablesCompsTotals, and SharedVariablesDataRep::variablesView.

14.254.3 Member Data Documentation

14.254.3.1 SizetArray variablesCompsTotals [private]

totals for variable type counts for {continuous,discrete integer,discrete string,discrete real} {design,aleatory uncertain,epistemic uncertain,state}.

This data reflects the variable counts as originally specified and is not altered by relaxation.

Referenced by SharedVariablesDataRep::aleatory_uncertain_counts(), SharedVariablesDataRep::all_counts(), SharedVariablesDataRep::components_to_totals(), SharedVariablesDataRep::copy_rep(), SharedVariablesDataRep::design_counts(), SharedVariablesDataRep::epistemic_uncertain_counts(), SharedVariablesDataRep::initialize_active_components(), SharedVariablesDataRep::initialize_all_ids(), SharedVariablesDataRep::initialize_components_totals(), SharedVariablesDataRep::initialize_inactive_components(), SharedVariablesDataRep::relax_noncategorical(), SharedVariablesDataRep::state_counts(), SharedVariablesDataRep::uncertain_counts(), and SharedVariablesDataRep::view_start_counts().

14.254.3.2 SizetArray activeVarsCompsTotals [private]

totals for active variable type counts for {continuous,discrete integer,discrete string,discrete real} {design,aleatory uncertain,epistemic uncertain,state}.

This data reflects the variable counts as originally specified and is not altered by relaxation.

Referenced by SharedVariablesDataRep::copy_rep(), and SharedVariablesDataRep::initialize_active_components().

14.254.3.3 SizetArray inactiveVarsCompsTotals [private]

totals for inactive variable type counts for {continuous,discrete integer,discrete string,discrete real} {design,aleatory uncertain,epistemic uncertain,state}.

This data reflects the variable counts as originally specified and is not altered by relaxation.

Referenced by SharedVariablesDataRep::copy_rep(), and SharedVariablesDataRep::initialize_inactive_components().

14.254.3.4 SizetMultiArray allContinuousIds [private]

array of 1-based position identifiers for the all continuous variables array

These identifiers define positions of the all continuous variables array within the total variable sequence. A primary use case is for defining derivative ids (DVV) based on an active subset.

Referenced by SharedVariablesDataRep::copy_rep(), and SharedVariablesDataRep::initialize_all_ids().

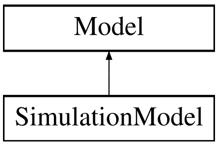
The documentation for this class was generated from the following files:

- SharedVariablesData.hpp
- SharedVariablesData.cpp

14.255 SimulationModel Class Reference

Derived model class which utilizes a simulation-based application interface to map variables into responses.

Inheritance diagram for SimulationModel:



Public Member Functions

- SimulationModel (ProblemDescDB &problem_db)

  constructor
- ∼SimulationModel ()

  destructor

Protected Member Functions

- Interface & derived_interface ()

  Return the "default" or maximal ActiveSet for the model.
- size_t solution_levels (bool lwr_bnd=true) const

  return size of solnCntlCostMap, optionally enforcing lower bound of 1 solution level
- RealVector solution_level_costs () const

  return all cost estimates from solnCntlCostMap
- Real solution_level_cost () const

  return active cost estimate from solnCntlCostMap
- void solution_level_cost_index (size_t cost_index)

  activate entry in solnCntlCostMap
- size_t solution_level_cost_index () const

  return active entry in solnCntlCostMap
- short solution_control_variable_type () const

  return solnCntlVarType
- size_t solution_control_variable_index () const

  return solnCntlAVIndex
- size_t solution_control_discrete_variable_index () const

  return solnCntlADVIndex
- int solution_level_int_value () const

  return a discrete int variable value corresponding to solnCntlADVIndex
- String solution_level_string_value () const

  return a discrete string variable value corresponding to solnCntlADVIndex
- Real solution_level_real_value () const

  return a discrete real variable value corresponding to solnCntlADVIndex
- size_t cost_metadata_index () const

  return costMetadataIndex
- void derived_evaluate (const ActiveSet &set)

  portion of evaluate() specific to SimulationModel (invokes a synchronous map() on userDefinedInterface)
- void derived_evaluate_nowait (const ActiveSet &set)

  portion of evaluate_nowait() specific to SimulationModel (invokes an asynchronous map() on userDefinedInterface)
- const IntResponseMap & derived_synchronize ()

  portion of synchronize() specific to SimulationModel (invokes synch() on userDefinedInterface)
- const IntResponseMap & derived_synchronize_nowait ()

  portion of synchronize_nowait() specific to SimulationModel (invokes synch_nowait() on userDefinedInterface)
- short local_eval_synchronization ()

return userDefinedInterface synchronization setting

- int local_eval_concurrency ()

  return userDefinedInterface asynchronous evaluation concurrency

- bool derived_master_overload () const

  flag which prevents overloading the master with a multiprocessor evaluation (request forwarded to userDefined-Interface)

- IntIntPair estimate_partition_bounds (int max_eval_concurrency)

  estimate the minimum and maximum partition sizes that can be utilized by this Model

- void derived_init_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set up SimulationModel for parallel operations (request forwarded to userDefinedInterface)

- void derived_init_serial ()

  set up SimulationModel for serial operations (request forwarded to userDefinedInterface).

- void derived_set_communicators (ParLevLIter pl_iter, int max_eval_concurrency, bool recurse_flag=true)

  set active parallel configuration for the SimulationModel (request forwarded to userDefinedInterface)

- void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)

  Service userDefinedInterface job requests received from the master. Completes when a termination message is received from stop_servers().

- void stop_servers ()

  executed by the master to terminate userDefinedInterface server operations when SimulationModel iteration is complete.

- const String & interface_id () const

  return the userDefinedInterface identifier

- int derived_evaluation_id () const

  return the current evaluation id (simModelEvalCntr)

- bool evaluation_cache (bool recurse_flag=true) const

  return flag indicated usage of an evaluation cache by the SimulationModel (request forwarded to userDefinedInterface)

- bool restart_file (bool recurse_flag=true) const

  return flag indicated usage of a restart file by the SimulationModel (request forwarded to userDefinedInterface)

- void set_evaluation_reference ()

  set the evaluation counter reference points for the SimulationModel (request forwarded to userDefinedInterface)

- void fine_grained_evaluation_counters ()

  request fine-grained evaluation reporting within the userDefinedInterface

- void print_evaluation_summary (std::ostream &s, bool minimal_header=false, bool relative_count=true) const

  print the evaluation summary for the SimulationModel (request forwarded to userDefinedInterface)

- void eval_tag_prefix (const String &eval_id_str)

  set the hierarchical eval ID tag prefix

- ActiveSet default_interface_active_set ()

  Return the "default" or maximal ActiveSet for the userDefinedInterface.

- void declare_sources ()

  Declare this model's sources.

Private Member Functions

- void initialize_solution_control (const String &control, const RealVector &cost)

  process the solution level inputs to define solnCntlVarType, solnCntlCostMap, and solnCntl{AV,ADV}Index

- void initialize_solution_recovery (const String &cost_label)

  process the solution level inputs to define solnCntlVarType, solnCntlCostMap, and solnCntl{AV,ADV}Index

Private Attributes

- Interface userDefinedInterface

    the interface used for mapping variables to responses
- short solnCntlVarType

    type of the discrete variable that controls the set/range of solution levels
- size_t solnCntlADVIndex

    index of the discrete variable (within all view) that controls the set/range of solution levels
- size_t solnCntlAVIndex

    index of the discrete variable (within all variables / RandomVariables array) that controls the set/range of solution levels
- std::multimap< Real, size_t > solnCntlCostMap

    sorted array of relative costs associated with a set of solution levels
- size_t costMetadataIndex

    index of metadata label used for online cost recovery
- size_t simModelEvalCntr

    counter for calls to derived_evaluate()/derived_evaluate_nowait()
- IntIntMap simIdMap

    map from userDefinedInterface evaluation ids to SimulationModel ids (may differ in case where the same interface instance is shared by multiple models)
- IntResponseMap simResponseMap

    map of simulation-based responses returned by derived_synchronize() and derived_synchronize_nowait()

Additional Inherited Members

14.255.1 Detailed Description

Derived model class which utilizes a simulation-based application interface to map variables into responses.

The SimulationModel class is the simplest of the derived model classes. It provides the capabilities of the original Model class, prior to the development of surrogate and nested model extensions. The derived response computation and synchronization functions utilize an application interface to perform the function evaluations.

14.255.2 Member Function Documentation

14.255.2.1 Interface & derived_interface ( ) [inline], [protected], [virtual]

Return the "default" or maximal ActiveSet for the model.

return userDefinedInterface

Reimplemented from Model.

References SimulationModel::userDefinedInterface.

14.255.2.2 void eval_tag_prefix (const String & *eval_id_str*) [protected], [virtual]

set the hierarchical eval ID tag prefix

SimulationModel doesn't need to change the tagging, so just forward to Interface

Reimplemented from Model.

References Interface::eval_tag_prefix(), and SimulationModel::userDefinedInterface.

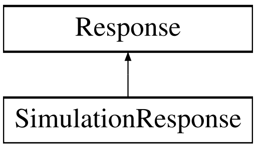
The documentation for this class was generated from the following files:

- SimulationModel.hpp
- SimulationModel.cpp

14.256 SimulationResponse Class Reference

Container class for response functions and their derivatives. SimulationResponse provides the body class.

Inheritance diagram for SimulationResponse:



Public Member Functions

- SimulationResponse ()

    default constructor
- SimulationResponse (const Variables &vars, const ProblemDescDB &problem_db)

    standard constructor built from problem description database
- SimulationResponse (const SharedResponseData &srd, const ActiveSet &set)

    alternate constructor that shares a SharedResponseData instance
- SimulationResponse (const SharedResponseData &srd)

    alternate constructor that shares a SharedResponseData instance
- SimulationResponse (const ActiveSet &set)

    alternate constructor using limited data
- ∼SimulationResponse ()

    destructor

Additional Inherited Members

14.256.1 Detailed Description

Container class for response functions and their derivatives. SimulationResponse provides the body class.

The SimulationResponse class is the "representation" of the response container class. It is the "body" portion of the "handle-body idiom" (see Coplien "Advanced C++", p. 58). The handle class (Response) provides for memory efficiency in management of multiple response objects through reference counting and representation sharing. The body class (SimulationResponse) actually contains the response data (functionValues, functionGradients, functionHessians, etc.). The representation is hidden in that an instance of SimulationResponse may only be created by Response. Therefore, programmers create instances of the Response handle class, and only need to be aware of the handle/body mechanisms when it comes to managing shallow copies (shared representation) versus deep copies (separate representation used for history mechanisms).

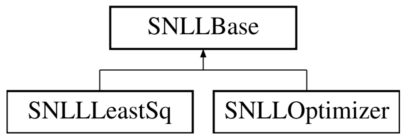
The documentation for this class was generated from the following files:

- SimulationResponse.hpp
- SimulationResponse.cpp

14.257 SNLLBase Class Reference

Base class for OPT++ optimization and least squares methods.

Inheritance diagram for SNLLBase:



Public Member Functions

- SNLLBase ()
  default constructor
- SNLLBase (ProblemDescDB &problem_db)
  standard constructor
- ∼SNLLBase ()
  destructor

Protected Member Functions

- void copy_con_vals_dak_to_optpp (const RealVector &local_fn_vals, RealVector &g, size_t offset)
  convenience function for copying local_fn_vals to g; used by constraint evaluator functions
- void copy_con_vals_optpp_to_dak (const RealVector &g, RealVector &local_fn_vals, size_t offset)
  convenience function for copying g to local_fn_vals; used in final solution logging
- void copy_con_grad (const RealMatrix &local_fn_grads, RealMatrix &grad_g, size_t offset)
  convenience function for copying local_fn_grads to grad_g; used by constraint evaluator functions
- void copy_con_hess (const RealSymMatrixArray &local_fn_hessians, OPTPP::OptppArray< RealSymMatrix > &hess_g, size_t offset)
  convenience function for copying local_fn_hessians to hess_g; used by constraint evaluator functions
- void snll_pre_instantiate (bool bound_constr_flag, int num_constr)
  convenience function for setting OPT++ options prior to the method instantiation
- void snll_post_instantiate (int num_cv, bool vendor_num_grad_flag, const String &finite_diff_type, const RealVector &fdss, size_t max_iter, size_t max_eval, Real conv_tol, Real grad_tol, Real max_step, bool bound_constr_flag, int num_constr, short output_lev, OPTPP::OptimizeClass ∗the_optimizer, OPTPP::NLP0 ∗nlf_objective, OPTPP::FDNLF1 ∗fd_nlf1, OPTPP::FDNLF1 ∗fd_nlf1_con)
  convenience function for setting OPT++ options after the method instantiation
- void snll_initialize_run (OPTPP::NLP0 ∗nlf_objective, OPTPP::NLP ∗nlp_constraint, const RealVector &init_pt, bool bound_constr_flag, const RealVector &lower_bnds, const RealVector &upper_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_targets, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_targets)
  convenience function for OPT++ configuration prior to the method invocation
- void snll_post_run (OPTPP::NLP0 ∗nlf_objective)
  convenience function for managing OPT++ results after method execution
- void snll_finalize_run (OPTPP::NLP0 ∗nlf_objective)
  convenience function for clearing OPT++ data after method execution
- void reset_base ()
  reset last{FnEvalLocn,EvalMode,EvalVars}

Static Protected Member Functions

- static void init_fn (int n, RealVector &x)
  An initialization mechanism provided by OPT++ (not currently used).

Protected Attributes

- String searchMethod

  value_based_line_search, gradient_based_line_search, trust_region, or tr_pds
- OPTPP::SearchStrategy searchStrat

  enum: LineSearch, TrustRegion, or TrustPDS
- OPTPP::MeritFcn meritFn

  enum: NormFmu, ArgaezTapia, or VanShanno
- Real maxStep

  value from `max_step` *specification*
- Real stepLenToBndry

  value from `steplength_to_boundary` *specification*
- Real centeringParam

  value from `centering_parameter` *specification*
- bool constantASVFlag

  flags a user selection of active_set_vector == constant. By mapping this into mode override, reliance on duplicate detection can be avoided.

Static Protected Attributes

- static Minimizer ∗ optLSqInstance

  pointer to the active base class object instance used within the static evaluator functions in order to avoid the need for static data
- static bool modeOverrideFlag

  flags OPT++ mode override (for combining value, gradient, and Hessian requests)
- static EvalType lastFnEvalLocn

  an enum used to track whether an nlf evaluator or a constraint evaluator was the last location of a function evaluation
- static int lastEvalMode

  copy of mode from constraint evaluators
- static RealVector lastEvalVars

  copy of variables from constraint evaluators

14.257.1 Detailed Description

Base class for OPT++ optimization and least squares methods.

The SNLLBase class provides a common base class for SNLLOptimizer and SNLLLeastSq, both of which are wrappers for OPT++, a C++ optimization library from the Computational Sciences and Mathematics Research (CS-MR) department at Sandia's Livermore CA site.

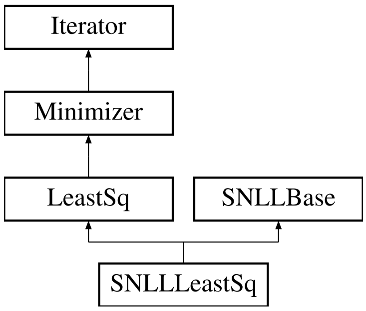
The documentation for this class was generated from the following files:

- SNLLBase.hpp
- SNLLBase.cpp

14.258 SNLLLeastSq Class Reference

Wrapper class for the OPT++ optimization library.

Inheritance diagram for SNLLLeastSq:



Public Member Functions

- SNLLLeastSq (ProblemDescDB &problem_db, Model &model)

  standard constructor
- SNLLLeastSq (const String &method_name, Model &model)

  alternate constructor for instantiations without ProblemDescDB support
- ∼SNLLLeastSq ()

  destructor
- void core_run ()

  compute the least squares solution
- void reset ()

  restore initial state for repeated sub-iterator executions

Protected Member Functions

- void initialize_run ()

  invokes LeastSq::initialize_run(), SNLLBase::snll_initialize_run(), and performs other set-up
- void finalize_run ()

  restores instances

Static Private Member Functions

- static void nlf2_evaluator_gn (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, RealSymMatrix &hess_f, int &result_mode)

  objective function evaluator function which obtains values and gradients for least square terms and computes objective function value, gradient, and Hessian using the Gauss-Newton approximation.
- static void constraint1_evaluator_gn (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)

  constraint evaluator function which provides constraint values and gradients to OPT++ Gauss-Newton methods.
- static void constraint2_evaluator_gn (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, OPTPP::OptppArray< RealSymMatrix > &hess_g, int &result_mode)

  constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ Gauss-Newton methods.

Private Attributes

- SNLLLeastSq ∗ prevSnllLSqInstance

  pointer to the previously active object instance used for restoration in the case of iterator/model recursion
- OPTPP::NLP0 ∗ nlfObjective

  objective NLF base class pointer

- OPTPP::NLP0 ∗ nlfConstraint

  constraint NLF base class pointer
- OPTPP::NLP ∗ nlpConstraint

  constraint NLP pointer
- OPTPP::NLF2 ∗ nlf2

  pointer to objective NLF for full Newton optimizers
- OPTPP::NLF2 ∗ nlf2Con

  pointer to constraint NLF for full Newton optimizers
- OPTPP::NLF1 ∗ nlf1Con

  pointer to constraint NLF for Quasi Newton optimizers
- OPTPP::OptimizeClass ∗ theOptimizer

  optimizer base class pointer
- OPTPP::OptNewton ∗ optnewton

  Newton optimizer pointer.
- OPTPP::OptBCNewton ∗ optbcnewton

  Bound constrained Newton optimizer ptr.
- OPTPP::OptDHNIPS ∗ optdhnips

  Disaggregated Hessian NIPS optimizer ptr.

Static Private Attributes

- static SNLLLeastSq ∗ snllLSqInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

14.258.1 Detailed Description

Wrapper class for the OPT++ optimization library.

The SNLLLeastSq class provides a wrapper for OPT++, a C++ optimization library of nonlinear programming and pattern search techniques from the Computational Sciences and Mathematics Research (CSMR) department at Sandia's Livermore CA site. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any attribute used within static member functions must be either local to that function, a static member, or accessed by static pointer.

The user input mappings are as follows: `max_iterations`, `max_function_evaluations`, `convergence_tolerance`, `max_step`, `gradient_tolerance`, `search_method`, and `search_scheme_size` are set using OPT++'s setMaxIter(), setMaxFeval(), setFcnTol(), setMaxStep(), setGradTol(), setSearchStrategy(), and setSSS() member functions, respectively; `output` verbosity is used to toggle OPT++'s debug mode using the setDebug() member function. Internal to OPT++, there are 3 search strategies, while the DAKOTA `search_method` specification supports 4 (`value_based_line_search`, `gradient_based_line_search`, `trust_region`, or `tr_pds`). The difference stems from the "is_expensive" flag in OPT++. If the search strategy is LineSearch and "is_expensive" is turned on, then the `value_based_line_search` is used. Otherwise (the "is_expensive" default is off), the algorithm will use the `gradient_based_line_search`. Refer to [Meza, J.C., 1994] and to the OPT++ source in the Dakota/packages/OPTPP directory for information on OPT++ class member functions.

14.258.2 Member Function Documentation

14.258.2.1 void nlf2_evaluator_gn (int *mode*, int *n*, const RealVector & *x*, double & *f*, RealVector & *grad_f*, RealSymMatrix & *hess_f*, int & *result_mode*) [static], [private]

objective function evaluator function which obtains values and gradients for least square terms and computes objective function value, gradient, and Hessian using the Gauss-Newton approximation.

This nlf2 evaluator function is used for the Gauss-Newton method in order to exploit the special structure of the nonlinear least squares problem. Here, fx = sum (T_i - Tbar_i)^2 and Response is made up of residual functions and their gradients along with any nonlinear constraints. The objective function and its gradient vector and Hessian matrix are computed directly from the residual functions and their derivatives (which are returned from the Response object).

References Dakota::abort_handler(), Iterator::activeSet, Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_values(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Minimizer::numFunctions, LeastSq::numLeastSqTerms, Minimizer::numNonlinearConstraints, Iterator::outputLevel, ActiveSet::request_vector(), SNLLLeastSq::snllLSqInstance, and Dakota::write_precision.

Referenced by SNLLLeastSq::SNLLLeastSq().

14.258.2.2 void constraint1_evaluator_gn (int *mode,* int *n,* const RealVector & *x,* RealVector & *g,* RealMatrix & *grad_g,* int & *result_mode*) [static], [private]

constraint evaluator function which provides constraint values and gradients to OPT++ Gauss-Newton methods.

While it does not employ the Gauss-Newton approximation, it is distinct from constraint1_evaluator() due to its need to anticipate the required modes for the least squares terms. This constraint evaluator function is used with diaggregated Hessian NIPS and is currently active.

References Dakota::abort_handler(), Iterator::activeSet, Model::continuous_variables(), SNLLBase::copy_con_grad(), SNLLBase::copy_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_values(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Minimizer::numFunctions, LeastSq::numLeastSqTerms, Iterator::outputLevel, ActiveSet::request_vector(), and SNLLLeastSq::snllLSqInstance.

Referenced by SNLLLeastSq::SNLLLeastSq().

14.258.2.3 void constraint2_evaluator_gn (int *mode,* int *n,* const RealVector & *x,* RealVector & *g,* RealMatrix & *grad_g,* OPTPP::OptppArray< RealSymMatrix > & *hess_g,* int & *result_mode*) [static], [private]

constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ Gauss-Newton methods.

While it does not employ the Gauss-Newton approximation, it is distinct from constraint2_evaluator() due to its need to anticipate the required modes for the least squares terms. This constraint evaluator function is used with full Newton NIPS and is currently inactive.

References Dakota::abort_handler(), Iterator::activeSet, Model::continuous_variables(), SNLLBase::copy_con_grad(), SNLLBase::copy_con_hess(), SNLLBase::copy_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_hessians(), Response::function_values(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, SNLLBase::modeOverrideFlag, Minimizer::numFunctions, LeastSq::numLeastSqTerms, Iterator::outputLevel, ActiveSet::request_vector(), and SNLLLeastSq::snllLSqInstance.

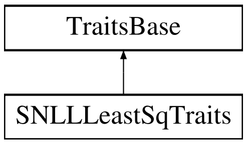
The documentation for this class was generated from the following files:

- SNLLLeastSq.hpp
- SNLLLeastSq.cpp

14.259 SNLLLeastSqTraits Class Reference

A version of TraitsBase specialized for SNLLLeastSq.

Inheritance diagram for SNLLLeastSqTraits:



Public Member Functions

- SNLLLeastSqTraits ()

  default constructor
- virtual ∼SNLLLeastSqTraits ()

  destructor
- virtual bool is_derived ()

  A temporary query used in the refactor.
- bool supports_continuous_variables ()

  Return the flag indicating whether method supports continuous variables.
- bool supports_linear_equality ()

  Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()

  Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()

  Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

  Return the flag indicating whether method supports nonlinear inequalities.

14.259.1 Detailed Description

A version of TraitsBase specialized for SNLLLeastSq.

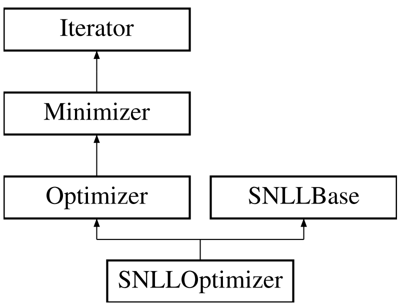
The documentation for this class was generated from the following file:

- SNLLLeastSq.hpp

14.260 SNLLOptimizer Class Reference

Wrapper class for the OPT++ optimization library.

Inheritance diagram for SNLLOptimizer:



Public Member Functions

- SNLLOptimizer (ProblemDescDB &problem_db, Model &model)

  standard constructor
- SNLLOptimizer (const String &method_string, Model &model)

  alternate constructor for instantiations "on the fly"
- SNLLOptimizer (const RealVector &initial_pt, const RealVector &var_l_bnds, const RealVector &var_u_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_tgts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, void(∗nlf1_obj_eval)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode), void(∗nlf1_con_eval)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode), size_t max_iter=100, size_t max_eval=1000, Real conv_tol=1.e-4, Real grad_tol=1.e-4, Real max_step=1000.)

  alternate constructor for objective/constraint call-backs; analytic gradient case
- SNLLOptimizer (const RealVector &initial_pt, const RealVector &var_l_bnds, const RealVector &var_u_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_tgts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, void(∗nlf0_obj_eval)(int n, const RealVector &x, double &f, int &result_mode), void(∗nlf1_con_eval)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode), size_t max_iter=100, size_t max_eval=1000, Real conv_tol=1.e-4, Real grad_tol=1.e-4, Real max_step=1000.)

  alternate constructor for objective/constraint call-backs; mixed gradient case: numerical objective, analytic constraints
- SNLLOptimizer (const RealVector &initial_pt, const RealVector &var_l_bnds, const RealVector &var_u_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_tgts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, void(∗nlf1_obj_eval)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode), void(∗nlf0_con_eval)(int n, const RealVector &x, RealVector &g, int &result_mode), size_t max_iter=100, size_t max_eval=1000, Real conv_tol=1.e-4, Real grad_tol=1.e-4, Real max_step=1000.)

  alternate constructor for objective/constraint call-backs; mixed gradient case: analytic objective, numerical constraints
- SNLLOptimizer (const RealVector &initial_pt, const RealVector &var_l_bnds, const RealVector &var_u_bnds, const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_tgts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, void(∗nlf0_obj_eval)(int n, const RealVector &x, double &f, int &result_mode), void(∗nlf0_con_eval)(int n, const RealVector &x, RealVector &g, int &result_mode), size_t max_iter=100, size_t max_eval=1000, Real conv_tol=1.e-4, Real grad_tol=1.e-4, Real max_step=1000.)

  alternate constructor for objective/constraint call-backs; numerical gradient case
- ∼SNLLOptimizer ()

  destructor
- void core_run ()

  Performs the iterations to determine the optimal solution.
- void reset ()

  restore initial state for repeated sub-iterator executions
- void declare_sources ()

  Declare sources to the evaluations database.
- void initial_point (const RealVector &pt)

  sets the initial point (active continuous variables) for this iterator (user-functions mode for which Model updating is not used)
- void variable_bounds (const RealVector &cv_lower_bnds, const RealVector &cv_upper_bnds)

  assign nonlinear inequality and equality constraint allowables for this iterator (user-functions mode for which Model updating is not used)
- void linear_constraints (const RealMatrix &lin_ineq_coeffs, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealMatrix &lin_eq_coeffs, const RealVector &lin_eq_targets)

assign linear inequality and linear equality constraints for this iterator (user-functions mode for which Model updating is not used)

- void nonlinear_constraints (const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_targets)

  assign nonlinear inequality and equality constraint allowables for this iterator (user-functions mode for which Model updating is not used)

Protected Member Functions

- void initialize_run ()

  invokes Optimizer::initialize_run(), SNLLBase::snll_initialize_run(), and performs other set-up
- void post_run (std::ostream &s)

  performs data recovery and calls Optimizer::post_run()
- void finalize_run ()

  performs cleanup, restores instances and calls parent finalize

Private Member Functions

- void default_instantiate_q_newton (void(∗obj_eval)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode))

  instantiate an OPTPP_Q_NEWTON solver using standard settings
- void default_instantiate_q_newton (void(∗obj_eval)(int n, const RealVector &x, double &f, int &result_mode))

  instantiate an OPTPP_Q_NEWTON solver using standard settings
- void default_instantiate_constraint (void(∗con_eval)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode))

  instantiate constraint objectives using standard settings
- void default_instantiate_constraint (void(∗con_eval)(int n, const RealVector &x, RealVector &g, int &result_mode))

  instantiate constraint objectives using standard settings
- void default_instantiate_newton (void(∗obj_eval)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, RealSymMatrix &hess_f, int &result_mode), void(∗con_eval)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, OPTPP::OptppArray< RealSymMatrix > &hess_g, int &result_mode))

  instantiate an OPTPP_NEWTON solver using standard settings

Static Private Member Functions

- static void nlf0_evaluator (int n, const RealVector &x, double &f, int &result_mode)

  objective function evaluator function for OPT++ methods which require only function values.
- static void nlf1_evaluator (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode)

  objective function evaluator function which provides function values and gradients to OPT++ methods.
- static void nlf2_evaluator (int mode, int n, const RealVector &x, double &f, RealVector &grad_f, RealSymMatrix &hess_f, int &result_mode)

  objective function evaluator function which provides function values, gradients, and Hessians to OPT++ methods.
- static void constraint0_evaluator (int n, const RealVector &x, RealVector &g, int &result_mode)

  constraint evaluator function for OPT++ methods which require only constraint values.
- static void constraint1_evaluator (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode)

  constraint evaluator function which provides constraint values and gradients to OPT++ methods.
- static void constraint2_evaluator (int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, OPTPP::OptppArray< RealSymMatrix > &hess_g, int &result_mode)

  constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ methods.

Private Attributes

- SNLLOptimizer ∗ prevSnllOptInstance

  pointer to the previously active object instance used for restoration in the case of iterator/model recursion
- OPTPP::NLP0 ∗ nlfObjective

  objective NLF base class pointer
- OPTPP::NLP0 ∗ nlfConstraint

  constraint NLF base class pointer
- OPTPP::NLP ∗ nlpConstraint

  constraint NLP pointer
- OPTPP::NLF0 ∗ nlf0

  pointer to objective NLF for nongradient optimizers
- OPTPP::NLF1 ∗ nlf1

  pointer to objective NLF for (analytic) gradient-based optimizers
- OPTPP::NLF1 ∗ nlf1Con

  pointer to constraint NLF for (analytic) gradient-based optimizers
- OPTPP::FDNLF1 ∗ fdnlf1

  pointer to objective NLF for (finite diff) gradient-based optimizers
- OPTPP::FDNLF1 ∗ fdnlf1Con

  pointer to constraint NLF for (finite diff) gradient-based optimizers
- OPTPP::NLF2 ∗ nlf2

  pointer to objective NLF for full Newton optimizers
- OPTPP::NLF2 ∗ nlf2Con

  pointer to constraint NLF for full Newton optimizers
- OPTPP::OptimizeClass ∗ theOptimizer

  optimizer base class pointer
- OPTPP::OptPDS ∗ optpds

  PDS optimizer pointer.
- OPTPP::OptCG ∗ optcg

  CG optimizer pointer.
- OPTPP::OptLBFGS ∗ optlbfgs

  L-BFGS optimizer pointer.
- OPTPP::OptNewton ∗ optnewton

  Newton optimizer pointer.
- OPTPP::OptQNewton ∗ optqnewton

  Quasi-Newton optimizer pointer.
- OPTPP::OptFDNewton ∗ optfdnewton

  Finite Difference Newton opt pointer.
- OPTPP::OptBCNewton ∗ optbcnewton

  Bound constrained Newton opt pointer.
- OPTPP::OptBCQNewton ∗ optbcqnewton

  Bnd constrained Quasi-Newton opt ptr.
- OPTPP::OptBCFDNewton ∗ optbcfdnewton

  Bnd constrained FD-Newton opt ptr.
- OPTPP::OptNIPS ∗ optnips

  NIPS optimizer pointer.
- OPTPP::OptQNIPS ∗ optqnips

  Quasi-Newton NIPS optimizer pointer.
- OPTPP::OptFDNIPS ∗ optfdnips

  Finite Difference NIPS opt pointer.
- String setUpType

flag for iteration mode: "model" (normal usage) or "user_functions" (user-supplied functions mode for "on the fly" instantiations). NonDReliability currently uses the user_functions mode.

- RealVector initialPoint

  initial point used in "user_functions" mode
- RealVector lowerBounds

  variable lower bounds used in "user_functions" mode
- RealVector upperBounds

  variable upper bounds used in "user_functions" mode
- RealMatrix linIneqCoeffs

  linear inequality constraint coefficients used in "user_functions" mode
- RealVector linIneqLowerBnds

  linear inequality constraint lower bounds used in "user_functions" mode
- RealVector linIneqUpperBnds

  linear inequality constraint upper bounds used in "user_functions" mode
- RealMatrix linEqCoeffs

  linear equality constraint coefficients used in "user_functions" mode
- RealVector linEqTargets

  linear equality constraint targets used in "user_functions" mode
- RealVector nlnIneqLowerBnds

  nonlinear inequality constraint lower bounds used in "user_functions" mode
- RealVector nlnIneqUpperBnds

  nonlinear inequality constraint upper bounds used in "user_functions" mode
- RealVector nlnEqTargets

  nonlinear equality constraint targets used in "user_functions" mode

Static Private Attributes

- static SNLLOptimizer * snllOptInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data

Additional Inherited Members

14.260.1 Detailed Description

Wrapper class for the OPT++ optimization library.

The SNLLOptimizer class provides a wrapper for OPT++, a C++ optimization library of nonlinear programming and pattern search techniques from the Computational Sciences and Mathematics Research (CSMR) department at Sandia's Livermore CA site. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any attribute used within static member functions must be either local to that function, a static member, or accessed by static pointer.

The user input mappings are as follows: `max_iterations`, `max_function_evaluations`, `convergence_tolerance`, `max_step`, `gradient_tolerance`, `search_method`, and `search_scheme_size` are set using OPT++'s setMaxIter(), setMaxFeval(), setFcnTol(), setMaxStep(), setGradTol(), setSearchStrategy(), and setSSS() member functions, respectively; `output` verbosity is used to toggle OPT++'s debug mode using the setDebug() member function. Internal to OPT++, there are 3 search strategies, while the DAKOTA `search_method` specification supports 4 (`value_based_line_search`, `gradient_based_line_search`, `trust_region`, or `tr_pds`). The difference stems from the "is_expensive" flag in OPT++. If the search strategy is LineSearch and "is_expensive" is turned on, then the `value_based_line_search` is used. Otherwise (the "is_expensive" default is off), the algorithm will use the `gradient_based_line_search`. Refer to [Meza, J.C., 1994] and to the OPT++ source in the Dakota/packages/OPTPP directory for information on OPT++ class member functions.

14.260.2 Constructor & Destructor Documentation

14.260.2.1 SNLLOptimizer (ProblemDescDB & *problem_db,* Model & *model*)

standard constructor

This constructor is used for normal instantiations using data from the ProblemDescDB.

References Dakota::abort_handler(), Minimizer::boundConstraintFlag, SNLLBase::centeringParam, SNLLOptimizer::constraint0_evaluator(), SNLLOptimizer::constraint1_evaluator(), SNLLOptimizer::constraint2_evaluator(), Iterator::convergenceTol, SNLLOptimizer::default_instantiate_constraint(), SNLLOptimizer::default_instantiate_newton(), SNLLOptimizer::default_instantiate_q_newton(), Model::fd_gradient_step_size(), SNLLOptimizer::fdnlf1, SNLLOptimizer::fdnlf1Con, ProblemDescDB::get_int(), ProblemDescDB::get_real(), SNLLBase::init_fn(), Model::interval_type(), Iterator::iteratedModel, Dakota::LARGE_SCALE, Iterator::maxEvalConcurrency, Iterator::maxFunctionEvals, Iterator::maxIterations, SNLLBase::maxStep, SNLLBase::meritFn, Iterator::method_enum_to_string(), Iterator::methodName, SNLLOptimizer::nlf0, SNLLOptimizer::nlf0_evaluator(), SNLLOptimizer::nlf1, SNLLOptimizer::nlf1_evaluator(), SNLLOptimizer::nlf1Con, SNLLOptimizer::nlf2_evaluator(), SNLLOptimizer::nlfConstraint, SNLLOptimizer::nlfObjective, SNLLOptimizer::nlpConstraint, Minimizer::numConstraints, Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, SNLLOptimizer::optbcfdnewton, SNLLOptimizer::optbcqnewton, SNLLOptimizer::optcg, SNLLOptimizer::optfdnewton, SNLLOptimizer::optfdnips, SNLLOptimizer::optlbfgs, SNLLOptimizer::optpds, SNLLOptimizer::optqnewton, SNLLOptimizer::optqnips, Iterator::outputLevel, Iterator::probDescDB, SNLLBase::searchStrat, SNLLBase::snll_post_instantiate(), SNLLBase::snll_pre_instantiate(), SNLLBase::stepLenToBndry, SNLLOptimizer::theOptimizer, and Minimizer::vendorNumericalGradFlag.

14.260.2.2 SNLLOptimizer (const String & *method_string,* Model & *model*)

alternate constructor for instantiations "on the fly"

This is an alternate constructor for instantiations on the fly using a Model but no ProblemDescDB.

References Dakota::abort_handler(), Minimizer::boundConstraintFlag, SNLLOptimizer::constraint1_evaluator(), SNLLOptimizer::constraint2_evaluator(), Iterator::convergenceTol, SNLLOptimizer::default_instantiate_constraint(), SNLLOptimizer::default_instantiate_newton(), SNLLOptimizer::default_instantiate_q_newton(), Model::fd_gradient_step_size(), Model::interval_type(), Iterator::iteratedModel, Iterator::maxFunctionEvals, Iterator::maxIterations, Iterator::method_enum_to_string(), Iterator::methodName, SNLLOptimizer::nlf1_evaluator(), SNLLOptimizer::nlf2_evaluator(), SNLLOptimizer::nlfObjective, Minimizer::numConstraints, Minimizer::numContinuousVars, Iterator::outputLevel, SNLLBase::snll_post_instantiate(), SNLLBase::snll_pre_instantiate(), SNLLOptimizer::theOptimizer, and Minimizer::vendorNumericalGradFlag.

14.260.2.3 SNLLOptimizer (const RealVector & *initial_pt,* const RealVector & *var_l_bnds,* const RealVector & *var_u_bnds,* const RealMatrix & *lin_ineq_coeffs,* const RealVector & *lin_ineq_l_bnds,* const RealVector & *lin_ineq_u_bnds,* const RealMatrix & *lin_eq_coeffs,* const RealVector & *lin_eq_tgts,* const RealVector & *nln_ineq_l_bnds,* const RealVector & *nln_ineq_u_bnds,* const RealVector & *nln_eq_tgts,* void(*)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode) *nlf1_obj_eval,* void(*)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode) *nlf1_con_eval,* size_t *max_iter* = 100*,* size_t *max_eval* = 1000*,* Real *conv_tol* = 1.e-4*,* Real *grad_tol* = 1.e-4*,* Real *max_step* = 1000.)

alternate constructor for objective/constraint call-backs; analytic gradient case

This is an alternate constructor for performing an optimization using the passed in objective function and constraint function pointers.

References Minimizer::bigRealBoundSize, Minimizer::boundConstraintFlag, Dakota::copy_data(), SNLLOptimizer::default_instantiate_constraint(), SNLLOptimizer::default_instantiate_q_newton(), SNLLOptimizer::initialPoint, SNLLOptimizer::lowerBounds, SNLLOptimizer::nlfObjective, Minimizer::numConstraints, Minimizer::numContinuousVars, Iterator::outputLevel, SNLLBase::snll_post_instantiate(), SNLLBase::snll_pre_instantiate(), SNLLOptimizer::theOptimizer, and SNLLOptimizer::upperBounds.

14.260.2.4 SNLLOptimizer (const RealVector & *initial_pt*, const RealVector & *var_l_bnds*, const RealVector & *var_u_bnds*, const RealMatrix & *lin_ineq_coeffs*, const RealVector & *lin_ineq_l_bnds*, const RealVector & *lin_ineq_u_bnds*, const RealMatrix & *lin_eq_coeffs*, const RealVector & *lin_eq_tgts*, const RealVector & *nln_ineq_l_bnds*, const RealVector & *nln_ineq_u_bnds*, const RealVector & *nln_eq_tgts*, void(∗)(int n, const RealVector &x, double &f, int &result_mode) *nlf0_obj_eval*, void(∗)(int mode, int n, const RealVector &x, RealVector &g, RealMatrix &grad_g, int &result_mode) *nlf1_con_eval*, size_t *max_iter* = `100`, size_t *max_eval* = `1000`, Real *conv_tol* = `1.e-4`, Real *grad_tol* = `1.e-4`, Real *max_step* = `1000.`)

alternate constructor for objective/constraint call-backs; mixed gradient case: numerical objective, analytic constraints

This is an alternate constructor for performing an optimization using the passed in objective function and constraint function pointers.

References Minimizer::bigRealBoundSize, Minimizer::boundConstraintFlag, Dakota::copy_data(), SNLLOptimizer::default_instantiate_constraint(), SNLLOptimizer::default_instantiate_q_newton(), SNLLOptimizer::initialPoint, SNLLOptimizer::lowerBounds, SNLLOptimizer::nlfObjective, Minimizer::numConstraints, Minimizer::numContinuousVars, Iterator::outputLevel, SNLLBase::snll_post_instantiate(), SNLLBase::snll_pre_instantiate(), SNLLOptimizer::theOptimizer, and SNLLOptimizer::upperBounds.

14.260.2.5 SNLLOptimizer (const RealVector & *initial_pt*, const RealVector & *var_l_bnds*, const RealVector & *var_u_bnds*, const RealMatrix & *lin_ineq_coeffs*, const RealVector & *lin_ineq_l_bnds*, const RealVector & *lin_ineq_u_bnds*, const RealMatrix & *lin_eq_coeffs*, const RealVector & *lin_eq_tgts*, const RealVector & *nln_ineq_l_bnds*, const RealVector & *nln_ineq_u_bnds*, const RealVector & *nln_eq_tgts*, void(∗)(int mode, int n, const RealVector &x, double &f, RealVector &grad_f, int &result_mode) *nlf1_obj_eval*, void(∗)(int n, const RealVector &x, RealVector &g, int &result_mode) *nlf0_con_eval*, size_t *max_iter* = `100`, size_t *max_eval* = `1000`, Real *conv_tol* = `1.e-4`, Real *grad_tol* = `1.e-4`, Real *max_step* = `1000.`)

alternate constructor for objective/constraint call-backs; mixed gradient case: analytic objective, numerical constraints

This is an alternate constructor for performing an optimization using the passed in objective function and constraint function pointers.

References Minimizer::bigRealBoundSize, Minimizer::boundConstraintFlag, Dakota::copy_data(), SNLLOptimizer::default_instantiate_constraint(), SNLLOptimizer::default_instantiate_q_newton(), SNLLOptimizer::initialPoint, SNLLOptimizer::lowerBounds, SNLLOptimizer::nlfObjective, Minimizer::numConstraints, Minimizer::numContinuousVars, Iterator::outputLevel, SNLLBase::snll_post_instantiate(), SNLLBase::snll_pre_instantiate(), SNLLOptimizer::theOptimizer, and SNLLOptimizer::upperBounds.

14.260.2.6 SNLLOptimizer (const RealVector & *initial_pt*, const RealVector & *var_l_bnds*, const RealVector & *var_u_bnds*, const RealMatrix & *lin_ineq_coeffs*, const RealVector & *lin_ineq_l_bnds*, const RealVector & *lin_ineq_u_bnds*, const RealMatrix & *lin_eq_coeffs*, const RealVector & *lin_eq_tgts*, const RealVector & *nln_ineq_l_bnds*, const RealVector & *nln_ineq_u_bnds*, const RealVector & *nln_eq_tgts*, void(∗)(int n, const RealVector &x, double &f, int &result_mode) *nlf0_obj_eval*, void(∗)(int n, const RealVector &x, RealVector &g, int &result_mode) *nlf0_con_eval*, size_t *max_iter* = `100`, size_t *max_eval* = `1000`, Real *conv_tol* = `1.e-4`, Real *grad_tol* = `1.e-4`, Real *max_step* = `1000.`)

alternate constructor for objective/constraint call-backs; numerical gradient case

This is an alternate constructor for performing an optimization using the passed in objective function and constraint function pointers.

References Minimizer::bigRealBoundSize, Minimizer::boundConstraintFlag, Dakota::copy_data(), SNLLOptimizer::default_instantiate_constraint(), SNLLOptimizer::default_instantiate_q_newton(), SNLLOptimizer::initialPoint, SNLLOptimizer::lowerBounds, SNLLOptimizer::nlfObjective, Minimizer::numConstraints, Minimizer::numContinuousVars, Iterator::outputLevel, SNLLBase::snll_post_instantiate(), SNLLBase::snll_pre_instantiate(), SNLLOptimizer::theOptimizer, and SNLLOptimizer::upperBounds.

14.260.3 Member Function Documentation

14.260.3.1 void nlf0_evaluator (int *n*, const RealVector & *x*, double & *f*, int & *result_mode*) [static], [private]

objective function evaluator function for OPT++ methods which require only function values.

For use when DAKOTA computes f and gradients are not directly available. This is used by nongradient-based optimizers such as PDS and by gradient-based optimizers in vendor numerical gradient mode (opt++'s internal finite difference routine is used).

References Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_value(), Iterator::iteratedModel, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Minimizer::numNonlinearConstraints, Iterator::outputLevel, Model::primary_response_fn_sense(), and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

14.260.3.2 void nlf1_evaluator (int *mode*, int *n*, const RealVector & *x*, double & *f*, RealVector & *grad_f*, int & *result_mode*) [static], [private]

objective function evaluator function which provides function values and gradients to OPT++ methods.

For use when DAKOTA computes f and df/dX (regardless of gradient type). Vendor numerical gradient case is handled by nlf0_evaluator.

References Iterator::activeSet, Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_gradient_copy(), Response::function_value(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Minimizer::numNonlinearConstraints, Iterator::outputLevel, Model::primary_response_fn_sense(), ActiveSet::request_values(), and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

14.260.3.3 void nlf2_evaluator (int *mode*, int *n*, const RealVector & *x*, double & *f*, RealVector & *grad_f*, RealSymMatrix & *hess_f*, int & *result_mode*) [static], [private]

objective function evaluator function which provides function values, gradients, and Hessians to OPT++ methods.

For use when DAKOTA receives f, df/dX, & d^2f/dx^2 from the ApplicationInterface (analytic only). Finite differencing does not make sense for a full Newton approach, since lack of analytic gradients & Hessian should dictate the use of quasi-newton or fd-newton. Thus, there is no fdnlf2_evaluator for use with full Newton approaches, since it is preferable to use quasi-newton or fd-newton with nlf1. Gauss-Newton does not fit this model; it uses nlf2_evaluator_gn instead of nlf2_evaluator.

References Iterator::activeSet, Model::continuous_variables(), Model::current_response(), Model::evaluate(), Response::function_gradient_copy(), Response::function_hessian(), Response::function_value(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Minimizer::numNonlinearConstraints, Iterator::outputLevel, Model::primary_response_fn_sense(), ActiveSet::request_values(), and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

14.260.3.4 void constraint0_evaluator (int *n*, const RealVector & *x*, RealVector & *g*, int & *result_mode*) [static], [private]

constraint evaluator function for OPT++ methods which require only constraint values.

For use when DAKOTA computes g and gradients are not directly available. This is used by nongradient-based optimizers and by gradient-based optimizers in vendor numerical gradient mode (opt++'s internal finite difference routine is used).

References Model::continuous_variables(), SNLLBase::copy_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response::function_values(), Iterator::iteratedModel, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Optimizer::numObjectiveFns, Iterator::outputLevel, and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

14.260.3.5 void constraint1_evaluator (int *mode*, int *n*, const RealVector & *x*, RealVector & *g*, RealMatrix & *grad_g*, int & *result_mode*) [static], [private]

constraint evaluator function which provides constraint values and gradients to OPT++ methods.

For use when DAKOTA computes g and dg/dX (regardless of gradient type). Vendor numerical gradient case is handled by constraint0_evaluator.

References Iterator::activeSet, Model::continuous_variables(), SNLLBase::copy_con_grad(), SNLLBase::copy-_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_values(), Iterator::iteratedModel, SNLLBase::lastEvalMode, SNLLBase::lastEvalVars, SN-LLBase::lastFnEvalLocn, Optimizer::numObjectiveFns, Iterator::outputLevel, ActiveSet::request_values(), and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

14.260.3.6 void constraint2_evaluator (int *mode*, int *n*, const RealVector & *x*, RealVector & *g*, RealMatrix & *grad_g*, OPTPP::OptppArray< RealSymMatrix > & *hess_g*, int & *result_mode*) [static], [private]

constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ methods.

For use when DAKOTA computes g, dg/dX, & d^2g/dx^2 (analytic only).

References Iterator::activeSet, Model::continuous_variables(), SNLLBase::copy_con_grad(), SNLLBase::copy_-con_hess(), SNLLBase::copy_con_vals_dak_to_optpp(), Model::current_response(), Model::evaluate(), Response-::function_gradients(), Response::function_hessians(), Response::function_values(), Iterator::iteratedModel, SNL-LBase::lastEvalMode, SNLLBase::lastEvalVars, SNLLBase::lastFnEvalLocn, Optimizer::numObjectiveFns, Iterator-::outputLevel, ActiveSet::request_values(), and SNLLOptimizer::snllOptInstance.

Referenced by SNLLOptimizer::SNLLOptimizer().

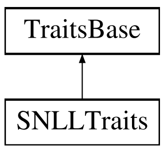
The documentation for this class was generated from the following files:

- SNLLOptimizer.hpp
- SNLLOptimizer.cpp

14.261 SNLLTraits Class Reference

A version of TraitsBase specialized for SNLL optimizers.

Inheritance diagram for SNLLTraits:



Public Member Functions

- SNLLTraits ()
  default constructor
- virtual ~SNLLTraits ()
  destructor
- virtual bool is_derived ()

A temporary query used in the refactor.

- bool supports_continuous_variables ()

    Return the value of supportsContinuousVariables.
- bool supports_linear_equality ()

    Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()

    Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()

    Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()

    Return the flag indicating whether method supports nonlinear inequalities.
- NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()

    Return the format used for nonlinear inequality constraints.

14.261.1 Detailed Description

A version of TraitsBase specialized for SNLL optimizers.

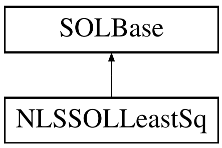
The documentation for this class was generated from the following file:

- SNLLOptimizer.hpp

14.262 SOLBase Class Reference

Base class for Stanford SOL software.

Inheritance diagram for SOLBase:



Public Member Functions

- SOLBase ()

    default constructor
- SOLBase (Model &model)

    standard constructor
- ∼SOLBase ()

    destructor

Protected Member Functions

- void check_sub_iterator_conflict (Model &model)

    check for clash with nested use of Fortran code
- void allocate_linear_arrays (int num_cv, const RealMatrix &lin_ineq_coeffs, const RealMatrix &lin_eq_coeffs)

    Allocates F77 linear constraint arrays for the SOL algorithms.
- void allocate_nonlinear_arrays (int num_cv, size_t num_nln_con)

    Allocates F77 nonlinear constraint arrays for the SOL algorithms.

- void size_bounds_array (size_t new_bnds_size)

  Updates arrays dependent on combined bounds size.
- void allocate_arrays (int num_cv, size_t num_nln_con, const RealMatrix &lin_ineq_coeffs, const RealMatrix &lin_eq_coeffs)

  Allocates F77 arrays for the SOL algorithms.
- void replace_linear_arrays (size_t num_cv, size_t num_nln_con, const RealMatrix &lin_ineq_coeffs, const RealMatrix &lin_eq_coeffs)

  update linear constraint arrays
- void replace_nonlinear_arrays (int num_cv, size_t num_lin_con, size_t num_nln_con)

  update nonlinear constraint arrays
- void deallocate_arrays ()

  Deallocates memory previously allocated by allocate_arrays().
- void allocate_workspace (int num_cv, int num_nln_con, int num_lin_con, int num_lsq)

  Allocates real and integer workspaces for the SOL algorithms.
- void set_options (bool speculative_flag, bool vendor_num_grad_flag, short output_lev, int verify_lev, Real fn_prec, Real linesrch_tol, size_t max_iter, Real constr_tol, Real conv_tol, const std::string &grad_type, const RealVector &fdss)

  Sets SOL method options using calls to npoptn2 / nloptn2.
- virtual void send_sol_option (std::string sol_option)=0

  Resize and send option to NPSOL (npoptn) or NLSSOL (nloptn) via derived implementation.
- void augment_bounds (RealVector &aggregate_l_bnds, RealVector &aggregate_u_bnds, const Model &model)

  augments variable bounds with linear and nonlinear constraint bounds.
- void augment_bounds (RealVector &aggregate_l_bnds, RealVector &aggregate_u_bnds, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealVector &lin_eq_targets, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_targets)

  augments variable bounds with linear and nonlinear constraint bounds.
- void replace_variable_bounds (size_t num_lin_con, size_t num_nln_con, RealVector &aggregate_l_bnds, RealVector &aggregate_u_bnds, const RealVector &cv_lower_bnds, const RealVector &cv_upper_bnds)

  replace variable bounds within aggregate arrays
- void replace_linear_bounds (size_t num_cv, size_t num_nln_con, RealVector &aggregate_l_bnds, RealVector &aggregate_u_bnds, const RealVector &lin_ineq_l_bnds, const RealVector &lin_ineq_u_bnds, const RealVector &lin_eq_targets)

  replace linear bounds within aggregate arrays
- void replace_nonlinear_bounds (size_t num_cv, size_t num_lin_con, RealVector &aggregate_l_bnds, RealVector &aggregate_u_bnds, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_targets)

  replace nonlinear bounds within aggregate arrays

Static Protected Member Functions

- static void constraint_eval (int &mode, int &ncnln, int &n, int &nrowj, int ∗needc, double ∗x, double ∗c, double ∗cjac, int &nstate)

  CONFUN in NPSOL manual: computes the values and first derivatives of the nonlinear constraint functions.

Protected Attributes

- int realWorkSpaceSize

  size of realWorkSpace
- int intWorkSpaceSize

  size of intWorkSpace
- RealArray realWorkSpace

real work space for NPSOL/NLSSOL

- IntArray intWorkSpace

  int work space for NPSOL/NLSSOL
- int nlnConstraintArraySize

  used for non-zero array sizing (nonlinear constraints)
- int linConstraintArraySize

  used for non-zero array sizing (linear constraints)
- RealArray cLambda

  CLAMBDA from NPSOL manual: Langrange multipliers.
- IntArray constraintState

  ISTATE from NPSOL manual: constraint status.
- int informResult

  INFORM from NPSOL manual: optimization status on exit.
- int numberIterations

  ITER from NPSOL manual: number of (major) iterations performed.
- int boundsArraySize

  length of aggregated bounds arrays (variable bounds plus linear and nonlinear constraint bounds)
- double ∗ linConstraintMatrixF77

  [A] matrix from NPSOL manual: linear constraint coefficients
- double ∗ upperFactorHessianF77

  [R] matrix from NPSOL manual: upper Cholesky factor of the Hessian of the Lagrangian.
- double ∗ constraintJacMatrixF77

  [CJAC] matrix from NPSOL manual: nonlinear constraint Jacobian
- int fnEvalCntr

  counter for testing against maxFunctionEvals
- size_t constrOffset

  used in constraint_eval() to bridge NLSSOLLeastSq::numLeastSqTerms and NPSOLOptimizer::numObjectiveFns

Static Protected Attributes

- static SOLBase ∗ solInstance

  pointer to the active object instance used within the static evaluator functions in order to avoid the need for static data
- static Minimizer ∗ optLSqInstance

  pointer to the active base class object instance used within the static evaluator functions in order to avoid the need for static data

14.262.1 Detailed Description

Base class for Stanford SOL software.

The SOLBase class provides a common base class for NPSOLOptimizer and NLSSOLLeastSq, both of which are Fortran 77 sequential quadratic programming algorithms from Stanford University marketed by Stanford Business Associates.

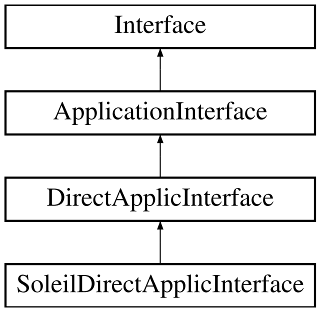
The documentation for this class was generated from the following files:

- SOLBase.hpp
- SOLBase.cpp

14.263 SoleilDirectApplicInterface Class Reference

Sample derived interface class for testing serial simulator plug-ins using assign_rep().

Inheritance diagram for SoleilDirectApplicInterface:



Public Member Functions

- SoleilDirectApplicInterface (const Dakota::ProblemDescDB &problem_db)

    constructor
- ∼SoleilDirectApplicInterface ()

    destructor

Protected Member Functions

- int derived_map_ac (const Dakota::String &ac_name)

    execute an analysis code portion of a direct evaluation invocation
- void derived_map_asynch (const Dakota::ParamResponsePair &pair)

    no-op hides base error; job batching occurs within wait_local_evaluations()
- void wait_local_evaluations (Dakota::PRPQueue &prp_queue)

    evaluate the batch of jobs contained in prp_queue
- void test_local_evaluations (Dakota::PRPQueue &prp_queue)

    invokes wait_local_evaluations() (no special nowait support)
- void set_communicators_checks (int max_eval_concurrency)

    no-op hides default run-time error checks at DirectApplicInterface level

Private Member Functions

- int rosenbrock (const Dakota::RealVector &c_vars, short asv, Dakota::Real &fn_val, Dakota::RealVector &fn-_grad, Dakota::RealSymMatrix &fn_hess)

    Rosenbrock plug-in test function.

Additional Inherited Members

14.263.1 Detailed Description

Sample derived interface class for testing serial simulator plug-ins using assign_rep().

The plug-in SoleilDirectApplicInterface resides in namespace SIM and uses a copy of rosenbrock() to perform serial parameter to response mappings. It is used to demonstrate plugging in a serial direct analysis driver into Dakota in library mode. Test input files can then use an analysis_driver of "plugin_rosenbrock".

14.263.2 Member Function Documentation

14.263.2.1 int derived_map_ac (const Dakota::String & *ac_name*) [protected], [virtual]

execute an analysis code portion of a direct evaluation invocation

Redefine this for serial/blocking execution of single Soleil simulations.

Reimplemented from DirectApplicInterface.

References Dakota::abort_handler(), ApplicationInterface::analysisServerId, DirectApplicInterface::directFnASV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, DirectApplicInterface::fnVals, ApplicationInterface::multiProcAnalysisFlag, SoleilDirectApplicInterface::rosenbrock(), and DirectApplicInterface::xC.

14.263.2.2 void wait_local_evaluations (Dakota::PRPQueue & *prp_queue*) [protected]

evaluate the batch of jobs contained in prp_queue

Redefine this for (Legion-based) execution of a batch of Soleil simulations. The incoming prp_queue is defined from ApplicationInterface::asynchLocalActivePRPQueue which is a local subset of beforeSynchCorePRPQueue. This function must complete at least one job (whereas test_local_evaluations() may complete zero). Populating completionSet results in decrementing the active queue and backfilling as indicated by concurrency level. For Soleil, we should not limit the concurrency level and will not combine with MPI scheduling –> incoming prp_queue is the full beforeSynchCorePRPQueue (no MPI distribution + no throttling). Further, we should complete the full local queue or we may need to distinguish still-running jobs from incoming new ones.

References Dakota::abort_handler(), ApplicationInterface::completionSet, Variables::continuous_variables(), Response::function_gradient_view(), Response::function_hessian_view(), Response::function_value_view(), ApplicationInterface::multiProcAnalysisFlag, Interface::outputLevel, ActiveSet::request_vector(), and SoleilDirectApplicInterface::rosenbrock().

Referenced by SoleilDirectApplicInterface::test_local_evaluations().

14.263.2.3 void test_local_evaluations (Dakota::PRPQueue & *prp_queue*) [inline], [protected]

invokes wait_local_evaluations() (no special nowait support)

For use by ApplicationInterface::serve_evaluations_asynch(), which can provide a batch processing capability within message passing schedulers (called using chain IteratorScheduler::run_iterator() –> Model::serve() –> ApplicationInterface::serve_evaluations() –> ApplicationInterface::serve_evaluations_asynch()).

References SoleilDirectApplicInterface::wait_local_evaluations().

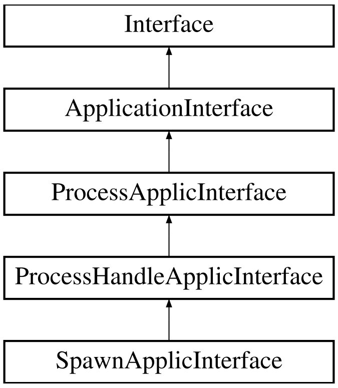
The documentation for this class was generated from the following files:

- SoleilDirectApplicInterface.hpp
- SoleilDirectApplicInterface.cpp

14.264 SpawnApplicInterface Class Reference

Derived application interface class which spawns simulation codes using spawnvp.

Inheritance diagram for SpawnApplicInterface:



Public Member Functions

- SpawnApplicInterface (const ProblemDescDB &problem_db)

    constructor
- ∼SpawnApplicInterface ()

    destructor

Protected Member Functions

- void wait_local_evaluation_sequence (PRPQueue &prp_queue)

    version of wait_local_evaluations() managing of set of individual asynchronous evaluations
- void test_local_evaluation_sequence (PRPQueue &prp_queue)

    version of test_local_evaluations() managing of set of individual asynchronous evaluations
- pid_t create_analysis_process (bool block_flag, bool new_group)

    spawn a child process for an analysis component within an evaluation
- size_t wait_local_analyses ()

    wait for asynchronous analyses on the local processor, completing at least one job
- size_t test_local_analyses_send (int analysis_id)

    test for asynchronous analysis completions on the local processor and return results for any completions by sending messages

Additional Inherited Members

14.264.1 Detailed Description

Derived application interface class which spawns simulation codes using spawnvp.

SpawnApplicInterface is used on Windows systems and is a peer to ForkApplicInterface for Unix systems.

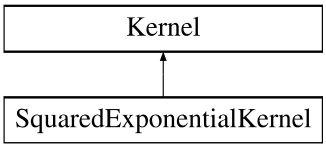
The documentation for this class was generated from the following files:

- SpawnApplicInterface.hpp
- SpawnApplicInterface.cpp

14.265 SquaredExponentialKernel Class Reference

Stationary kernel with C^ smooth realizations.

Inheritance diagram for SquaredExponentialKernel:



Public Member Functions

- void compute_gram (const std::vector< MatrixXd > &dists2, const VectorXd &theta_values, MatrixXd &gram) override

  Compute a Gram matrix given a vector of squared distances and kernel hyperparameters.
- void compute_gram_derivs (const MatrixXd &gram, const std::vector< MatrixXd > &dists2, const VectorXd &theta_values, std::vector< MatrixXd > &gram_derivs) override

  Compute the derivatives of the Gram matrix with respect to the kernel hyperparameters.
- MatrixXd compute_first_deriv_pred_gram (const MatrixXd &pred_gram, const std::vector< MatrixXd > &mixed_dists, const VectorXd &theta_values, const int index) override

  Compute the first derivatve of the prediction matrix for a given component.
- MatrixXd compute_second_deriv_pred_gram (const MatrixXd &pred_gram, const std::vector< MatrixXd > &mixed_dists, const VectorXd &theta_values, const int index_i, const int index_j) override

  Compute the second derivatve of the prediction matrix for a pair of components.

Additional Inherited Members

14.265.1 Detailed Description

Stationary kernel with C^ smooth realizations.

14.265.2 Member Function Documentation

14.265.2.1 void compute_gram (const std::vector< MatrixXd > & *dists2*, const VectorXd & *theta_values*, MatrixXd & *gram*) [override], [virtual]

Compute a Gram matrix given a vector of squared distances and kernel hyperparameters.

Parameters

in	*dists2*	Vector of squared distance matrices.
in	*theta_values*	Vector of hyperparameters.
in,out	*gram*	Gram matrix.

Returns

Gram matrix.

Implements Kernel.

References Kernel::compute_Dbar().

14.265.2.2 void compute_gram_derivs (const MatrixXd & *gram*, const std::vector< MatrixXd > & *dists2*, const VectorXd & *theta_values*, std::vector< MatrixXd > & *gram_derivs*) [override], [virtual]

Compute the derivatives of the Gram matrix with respect to the kernel hyperparameters.

Parameters

in	*gram*	Gram Matrix
in	*dists2*	Vector of squared distance matrices.
in	*theta_values*	Vector of hyperparameters.
in,out	*gram_derivs*	Vector of Gram matrix derivatives.

Returns

Derivatives of the Gram matrix w.r.t. the hyperparameters.

Implements Kernel.

14.265.2.3 MatrixXd compute_first_deriv_pred_gram (const MatrixXd & *pred_gram,* const std::vector< MatrixXd > & *mixed_dists,* const VectorXd & *theta_values,* const int *index*) [override], [virtual]

Compute the first derivatve of the prediction matrix for a given component.

Parameters

in	*pred_gram*	Prediction Gram matrix - Rectangular matrix of kernel evaluations between the surrogate and prediction points.
in	*mixed_dists*	Component-wise signed distances between the prediction and build points.
in	*theta_values*	Vector of hyperparameters.
in	*index*	Specifies the component of the derivative.

Returns

first_deriv_pred_gram First derivative of the prediction Gram matrix for a given component.

Implements Kernel.

14.265.2.4 MatrixXd compute_second_deriv_pred_gram (const MatrixXd & *pred_gram,* const std::vector< MatrixXd > & *mixed_dists,* const VectorXd & *theta_values,* const int *index_i,* const int *index_j*) [override], [virtual]

Compute the second derivatve of the prediction matrix for a pair of components.

Parameters

in	*pred_gram*	Prediction Gram matrix - Rectangular matrix of kernel evaluations between the surrogate and prediction points.
in	*mixed_dists*	Component-wise signed distances between the prediction and build points.
in	*theta_values*	Vector of hyperparameters.
in	*index_i*	Specifies the first component of the second derivative.
in	*index_j*	Specifies the second component of the second derivative.

Returns

second_deriv_pred_gram Second derivative of the prediction matrix for a pair of components.

Implements Kernel.

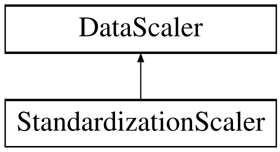
The documentation for this class was generated from the following files:

- SurrogatesGPKernels.hpp
- SurrogatesGPKernels.cpp

14.266 StandardizationScaler Class Reference

Standardizes the data so the each feature has zero mean and unit variance.

Inheritance diagram for StandardizationScaler:



Public Member Functions

- StandardizationScaler (const MatrixXd &features, double norm_factor=1.0)

    Main constructor for StandardizationScaler.

Additional Inherited Members

14.266.1 Detailed Description

Standardizes the data so the each feature has zero mean and unit variance.

scaler_offsets = mean

scale_factors = standard_deviation/norm_factor

14.266.2 Constructor & Destructor Documentation

14.266.2.1 StandardizationScaler (const MatrixXd & *features,* double *norm_factor* = `1.0`)

Main constructor for StandardizationScaler.

Parameters

in	*features*	Unscaled data matrix - (num_samples by num_features)
in	*norm_factor*	Optional scaling factor applied to each feature Has a default value of 1.0

References DataScaler::hasScaling, DataScaler::scaledSample, DataScaler::scalerFeaturesOffsets, and DataScaler::scalerFeaturesScaleFactors.

The documentation for this class was generated from the following files:

- UtilDataScaler.hpp
- UtilDataScaler.cpp

14.267 StringScale Struct Reference

Data structure for storing string-valued dimension scale.

Public Member Functions

- StringScale (const std::string &in_label, const char *const in_items[], const int &len, ScaleScope in_scope=ScaleScope::UNSHARED)

Constructor that takes a C-style array of C-strings.

- StringScale (const std::string &in_label, std::initializer_list< const char ∗ > in_items, ScaleScope in_-scope=ScaleScope::UNSHARED)

  Constructor that takes and initializer list of string literals.

- StringScale (const std::string &in_label, const std::vector< String > &in_items, ScaleScope in_scope=Scale-Scope::UNSHARED)

  Constructor that takes a vector of strings.

- StringScale (const std::string &in_label, std::vector< const char ∗ > in_items, ScaleScope in_scope=Scale-Scope::UNSHARED)

  Constructor that takes a vector of C-style strings.

- StringScale (const std::string &in_label, const StringMultiArrayConstView in_items, ScaleScope in_-scope=ScaleScope::UNSHARED)

  Constructor that takes a StringMultiArrayConstView.

- StringScale (const std::string &in_label, const std::vector< String > &in_items, const size_t first, const size_t num, ScaleScope in_scope=ScaleScope::UNSHARED)

  Constructor that takes indexes into a StringArray.

- StringScale (const std::string &in_label, std::vector< std::vector< const char ∗ > > in_items, ScaleScope in_scope=ScaleScope::UNSHARED)

  Constructor that takes a vector<vector<const char ∗> > to produce a 2D scale.

Public Attributes

- std::string label

  Scale label.

- ScaleScope scope

  Scale scope (whether the scaled is shared among responses)

- std::vector< const char ∗ > items

  Pointers to the strings that make up the scale.

- int numCols

  Number of columns; equals length of scale when 1D.

- bool isMatrix

  2d or 1d?

14.267.1 Detailed Description

Data structure for storing string-valued dimension scale.

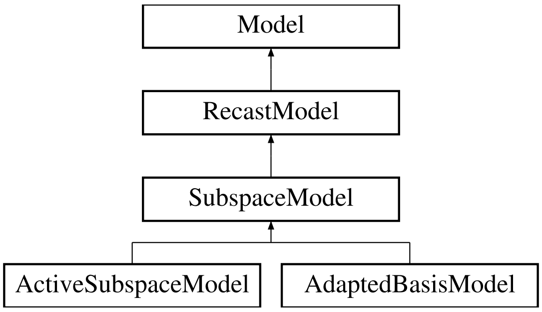
The documentation for this struct was generated from the following file:

- dakota_results_types.hpp

14.268 SubspaceModel Class Reference

Subspace model for input (variable space) reduction.

Inheritance diagram for SubspaceModel:



Public Member Functions

- SubspaceModel (ProblemDescDB &problem_db, const Model &sub_model)
  Problem database constructor.
- SubspaceModel (const Model &sub_model, unsigned int dimension, short output_level)
  lightweight constructor
- ∼SubspaceModel ()
  destructor
- bool initialize_mapping (ParLevLIter pl_iter)
- bool resize_pending () const
  return true if a potential resize is still pending, such that sizing-based initialization should be deferred
- void stop_init_mapping (ParLevLIter pl_iter)
  called from IteratorScheduler::init_iterator() for iteratorComm rank 0 to terminate serve_init_mapping() on other iteratorComm processors
- int serve_init_mapping (ParLevLIter pl_iter)
  called from IteratorScheduler::init_iterator() for iteratorComm rank != 0 to balance resize() calls on iteratorComm rank 0
- const RealMatrix & reduced_basis () const
  return reducedBasis

Protected Member Functions

- void derived_evaluate (const ActiveSet &set)
  portion of evaluate() specific to RecastModel (forward to subModel.evaluate())
- void derived_evaluate_nowait (const ActiveSet &set)
  portion of evaluate_nowait() specific to RecastModel (forward to subModel.evaluate_nowait())
- const IntResponseMap & derived_synchronize ()
  portion of synchronize() specific to RecastModel (forward to subModel.synchronize())
- const IntResponseMap & derived_synchronize_nowait ()
  portion of synchronize_nowait() specific to RecastModel (forward to subModel.synchronize_nowait())
- void component_parallel_mode (short mode)
  update component parallel mode for supporting parallelism in the offline and online phases
- void serve_run (ParLevLIter pl_iter, int max_eval_concurrency)
  Service the offline and online phase job requests received from the master; completes when termination message received from stop_servers().
- void stop_servers ()
  Executed by the master to terminate the offline and online phase server operations when iteration on the SubspaceModel is complete.
- void assign_instance ()
  assign static pointer instance to this for use in static transformation functions
- virtual void validate_inputs ()

validate the build controls and set defaults

- virtual void compute_subspace ()=0

  sample the model's gradient, computed the SVD, and form the active subspace rotation matrix.
- virtual void initialize_subspace ()

  helper for shared code between lightweight ctor and initialize_mapping()
- virtual void uncertain_vars_to_subspace ()

  translate the characterization of uncertain variables in the native_model to the reduced space of the transformed model
- void initialize_base_recast (void(∗variables_map)(const Variables &recast_vars, Variables &sub_model_vars), void(∗set_map)(const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set), void(∗primary_resp_map)(const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &recast_response))

  Initialize the base class RecastModel with reduced space variable sizes.
- SizetArray resize_variable_totals ()

  Create a variables components totals array with the reduced space size for continuous variables.
- void update_linear_constraints ()

  transform the original bounded domain (and any existing linear constraints) into linear constraints in the reduced space
- void update_var_labels ()

  update variable labels

Static Protected Member Functions

- static void set_mapping (const Variables &recast_vars, const ActiveSet &recast_set, ActiveSet &sub_model_set)

  map the inbound ActiveSet to the sub-model (map derivative variables)
- static void response_mapping (const Variables &recast_y_vars, const Variables &sub_model_x_vars, const Response &sub_model_resp, Response &recast_resp)

  map responses from the sub-model to the recast model

Protected Attributes

- int randomSeed

  seed controlling all samplers
- size_t numFullspaceVars

  Number of fullspace active continuous variables.
- unsigned int reducedRank

  current approximation of system rank
- RealMatrix reducedBasis

  basis for the reduced subspace
- size_t miPLIndex

  the index of the active metaiterator-iterator parallelism level (corresponding to ParallelConfiguration::miPLIters) used at runtime
- int onlineEvalConcurrency

  Concurrency to use once subspace has been built.
- int offlineEvalConcurrency

  Concurrency to use when building subspace.

Static Protected Attributes

- static SubspaceModel ∗ smInstance

  static pointer to this class for use in static member fn callbacks

Additional Inherited Members

14.268.1 Detailed Description

Subspace model for input (variable space) reduction.

Specialization of a RecastModel that identifies a subspace during build phase and creates a RecastModel in the reduced space

14.268.2 Member Function Documentation

14.268.2.1 bool initialize_mapping (ParLevLIter *pl_iter*) [virtual]

May eventually take on init_comms and related operations. Also may want ide of build/update like DataFitSurrModel, eventually.

Reimplemented from RecastModel.

References SubspaceModel::component_parallel_mode(), SubspaceModel::compute_subspace(), RecastModel::initialize_mapping(), SubspaceModel::initialize_subspace(), SubspaceModel::miPLIndex, Model::modelPCIter, SubspaceModel::numFullspaceVars, and SubspaceModel::reducedRank.

14.268.2.2 void derived_evaluate (const ActiveSet & *set*) [protected], [virtual]

portion of evaluate() specific to RecastModel (forward to subModel.evaluate())

The RecastModel is evaluated by an Iterator for a recast problem formulation. Therefore, the currentVariables, incoming active set, and output currentResponse all correspond to the recast inputs/outputs.

Reimplemented from RecastModel.

References Dakota::abort_handler(), SubspaceModel::component_parallel_mode(), RecastModel::derived_evaluate(), and Model::mappingInitialized.

14.268.2.3 void uncertain_vars_to_subspace ( ) [protected], [virtual]

translate the characterization of uncertain variables in the native_model to the reduced space of the transformed model

Convert the user-specified normal random variables to the appropriate reduced space variables, based on the orthogonal transformation.

TODO: Generalize to convert other random variable types (non-normal)

TODO: The translation of the correlations from full to reduced space is likely wrong for rank correlations; should be correct for covariance.

Reimplemented in ActiveSubspaceModel, and AdaptedBasisModel.

References Dakota::abort_handler(), Model::current_variables(), SharedVariablesData::cv_index_to_all_index(), Model::multivariate_distribution(), Model::mvDist, SubspaceModel::numFullspaceVars, SubspaceModel::reducedRank, Variables::shared_data(), RecastModel::subModel, and Dakota::svd().

Referenced by SubspaceModel::initialize_subspace(), AdaptedBasisModel::uncertain_vars_to_subspace(), and ActiveSubspaceModel::uncertain_vars_to_subspace().

14.268.2.4 void initialize_base_recast (void(*)(const **Variables** &recast_vars, **Variables** &sub_model_vars) *variables_map*, void(*)(const **Variables** &recast_vars, const **ActiveSet** &recast_set, **ActiveSet** &sub_model_set) *set_map*, void(*)(const **Variables** &sub_model_vars, const **Variables** &recast_vars, const **Response** &sub_model_response, **Response** &recast_response) *primary_resp_map*) [protected]

Initialize the base class RecastModel with reduced space variable sizes.

Initialize the recast model based on the reduced space, with no response function mapping (for now). TODO: use a surrogate model over the inactive dimension.

References Model::current_response(), Model::cv(), Model::div(), Model::drv(), Model::dsv(), Response::function_gradients(), Response::function_hessians(), RecastModel::init_maps(), RecastModel::init_sizes(), Model::num_nonlinear_ineq_constraints(), Model::num_primary_fns(), Model::num_secondary_fns(), Model::numFns, SubspaceModel::reducedRank, SubspaceModel::resize_variable_totals(), and RecastModel::subModel.

Referenced by AdaptedBasisModel::uncertain_vars_to_subspace(), and ActiveSubspaceModel::uncertain_vars_to_subspace().

14.268.2.5 void set_mapping (const **Variables** & *reduced_vars*, const **ActiveSet** & *reduced_set*, **ActiveSet** & *full_set*) [static], [protected]

map the inbound ActiveSet to the sub-model (map derivative variables)

Simplified derivative variables mapping where all continuous depend on all others. TODO: Could instead rely on a richer default in RecastModel based on varsMapIndices.

References Variables::cv(), ActiveSet::derivative_vector(), SubspaceModel::numFullspaceVars, and SubspaceModel::smInstance.

Referenced by AdaptedBasisModel::uncertain_vars_to_subspace(), and ActiveSubspaceModel::uncertain_vars_to_subspace().

14.268.2.6 void response_mapping (const **Variables** & *reduced_vars*, const **Variables** & *full_vars*, const **Response** & *full_resp*, **Response** & *reduced_resp*) [static], [protected]

map responses from the sub-model to the recast model

Perform the response mapping from submodel to recast response

References Response::function_gradients(), Response::function_hessians(), Response::function_values(), SubspaceModel::reducedBasis, and SubspaceModel::smInstance.

Referenced by AdaptedBasisModel::uncertain_vars_to_subspace(), and ActiveSubspaceModel::uncertain_vars_to_subspace().

14.268.3 Member Data Documentation

14.268.3.1 **SubspaceModel** * smInstance [static], [protected]

static pointer to this class for use in static member fn callbacks

initialization of static needed by RecastModel callbacks

Referenced by SubspaceModel::assign_instance(), SubspaceModel::response_mapping(), SubspaceModel::set_mapping(), and AdaptedBasisModel::variables_mapping().

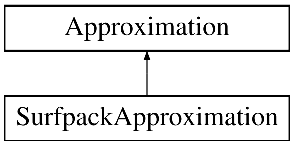
The documentation for this class was generated from the following files:

- SubspaceModel.hpp
- SubspaceModel.cpp

14.269 SurfpackApproximation Class Reference

Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.

Inheritance diagram for SurfpackApproximation:



Public Member Functions

- SurfpackApproximation ()

  default constructor
- SurfpackApproximation (const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

  standard constructor: Surfpack surface of appropriate type will be created
- SurfpackApproximation (const SharedApproxData &shared_data)

  alternate constructor
- ~SurfpackApproximation ()

  destructor

Protected Member Functions

- int min_coefficients () const override

  return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- int recommended_coefficients () const override

  return the recommended number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- void build () override

  SurfData object will be created from Dakota's SurrogateData, and the appropriate Surfpack build method will be invoked.
- void map_variable_labels (const Variables &vars)

  validate imported labels and initialize map if needed
- void export_model (const StringArray &var_labels, const String &fn_label, const String &export_prefix, const unsigned short export_format) override

  export the Surpack model to disk or console
- void export_model (const Variables &vars, const String &fn_label, const String &export_prefix, const unsigned short export_format) override

  approximation export that generates labels from the passed Variables, since only the derived classes know how the variables are ordered w.r.t. the surrogate build; if export_format > NO_MODEL_FORMAT, uses all 3 parameters, otherwise extracts these from the Approximation's sharedDataRep to build a filename
- Real value (const Variables &vars) override

  Return the value of the Surfpack surface for a given parameter vector x.
- const RealVector & gradient (const Variables &vars) override

  retrieve the approximate function gradient for a given parameter vector x
- const RealSymMatrix & hessian (const Variables &vars) override

  retrieve the approximate function Hessian for a given parameter vector x
- Real prediction_variance (const Variables &vars) override

retrieve the variance of the predicted value for a given parameter set x (KrigingModel only)

- Real value (const RealVector &c_vars) override

  Return the value of the Surfpack surface for a given parameter vector x.

- const RealVector & gradient (const RealVector &c_vars) override

  retrieve the approximate function gradient for a given parameter vector x

- const RealSymMatrix & hessian (const RealVector &c_vars) override

  retrieve the approximate function Hessian for a given parameter vector x

- Real prediction_variance (const RealVector &c_vars) override

  retrieve the variance of the predicted value for a given parameter set x (KrigingModel only)

- bool diagnostics_available () override

  check if the diagnostics are available (true for the Surfpack types)

- Real diagnostic (const String &metric_type) override

  retrieve a single diagnostic metric for the diagnostic type specified on the primary model and data

- Real diagnostic (const String &metric_type, const SurfpackModel &model, const SurfData &data)

  retrieve a single diagnostic metric for the diagnostic type specified on the given model and data - not inherited

- void primary_diagnostics (size_t fn_index) override

  compute and print all requested diagnostics and cross-validation

- void challenge_diagnostics (size_t fn_index, const RealMatrix &challenge_points, const RealVector &challenge_responses) override

  compute and print all requested diagnostics for user provided challenge pts

- RealArray cv_diagnostic (const StringArray &metric_types, unsigned num_folds) override

  compute and return cross-validation for metric_type with num_folds

- RealArray challenge_diagnostic (const StringArray &metric_types, const RealMatrix &challenge_points, const RealVector &challenge_responses) override

  compute and print all requested diagnostics for user provided challenge pts

Private Member Functions

- void import_model (const ProblemDescDB &problem_db)

  construct-time only import of serialized surrogate

- void surrogates_to_surf_data ()

  copy from SurrogateData to SurfPoint/SurfData in surfData

- void add_constraints_to_surfdata (const Pecos::SurrogateDataVars &anchor_vars, const Pecos::SurrogateDataResp &anchor_resp, short fail_code)

  set the anchor point (including gradient and hessian if present) into surf_data

- RealArray map_eval_vars (const Variables &vars)

  extract active or all view as vector, mapping if needed for import

Private Attributes

- std::shared_ptr< SurfpackModel > spModel

  The native Surfpack approximation.

- std::shared_ptr
  < SurfpackModelFactory > spFactory

  factory for the SurfpackModel instance

- std::shared_ptr< SurfData > surfData

  The data used to build the approximation, in Surfpack format.

- bool modelIsImported

  whether model serialized in from disk

Additional Inherited Members

14.269.1 Detailed Description

Derived approximation class for Surfpack approximation classes. Interface between Surfpack and Dakota.

The SurfpackApproximation class is the interface between Dakota and Surfpack. Based on the information in the ProblemDescDB that is passed in through the constructor, SurfpackApproximation builds a Surfpack Surface object that corresponds to one of the following data-fitting techniques: polynomial regression, kriging, artificial neural networks, radial basis function network, or multivariate adaptaive regression splines (MARS).

14.269.2 Constructor & Destructor Documentation

14.269.2.1 SurfpackApproximation (const ProblemDescDB & *problem_db,* const SharedApproxData & *shared_data,* const String & *approx_label*)

standard constructor: Surfpack surface of appropriate type will be created

Initialize the embedded Surfpack surface object and configure it using the specifications from the input file. Data for the surface is created later.

References Dakota::abort_handler(), Dakota::copy_data(), ProblemDescDB::get_bool(), ProblemDescDB::get_real(), ProblemDescDB::get_rv(), ProblemDescDB::get_short(), ProblemDescDB::get_string(), SurfpackApproximation::import_model(), Approximation::sharedDataRep, and SurfpackApproximation::spFactory.

14.269.2.2 SurfpackApproximation (const SharedApproxData & *shared_data*)

alternate constructor

On-the-fly constructor which uses mostly Surfpack model defaults.

References Dakota::abort_handler(), Approximation::sharedDataRep, and SurfpackApproximation::spFactory.

14.269.3 Member Function Documentation

14.269.3.1 void build ( ) [override], [protected], [virtual]

SurfData object will be created from Dakota's SurrogateData, and the appropriate Surfpack build method will be invoked.

Todo Right now, we're completely deleting the old data and then recopying the current data into a SurfData object. This was just the easiest way to arrive at a solution that would build and run. This function is frequently called from addPoint rebuild, however, and it's not good to go through this whole process every time one more data point is added.

Reimplemented from Approximation.

References Dakota::abort_handler(), Approximation::build(), SurfpackApproximation::modelIsImported, Approximation::sharedDataRep, SurfpackApproximation::spFactory, SurfpackApproximation::spModel, SurfpackApproximation::surfData, and SurfpackApproximation::surrogates_to_surf_data().

14.269.3.2 const RealSymMatrix & hessian (const Variables & *vars*) [override], [protected], [virtual]

retrieve the approximate function Hessian for a given parameter vector x

Todo Make this acceptably efficient

Reimplemented from Approximation.

References Dakota::abort_handler(), Approximation::approxHessian, Variables::cv(), SurfpackApproximation::map_eval_vars(), Approximation::sharedDataRep, and SurfpackApproximation::spModel.

Referenced by SurfpackApproximation::add_constraints_to_surfdata().

14.269.3.3 const RealSymMatrix & hessian (const RealVector & *c_vars*) [override], [protected], [virtual]

retrieve the approximate function Hessian for a given parameter vector x

Todo Make this acceptably efficient

Reimplemented from Approximation.

References Dakota::abort_handler(), Approximation::approxHessian, Approximation::sharedDataRep, and SurfpackApproximation::spModel.

14.269.3.4 void surrogates_to_surf_data ( ) [private]

copy from SurrogateData to SurfPoint/SurfData in surfData

Copy the data stored in Dakota-style SurrogateData into Surfpack-style SurfPoint and SurfData objects. Updates surfData

References SurfpackApproximation::add_constraints_to_surfdata(), Approximation::approxData, Approximation::sharedDataRep, SurfpackApproximation::spFactory, and SurfpackApproximation::surfData.

Referenced by SurfpackApproximation::build().

14.269.3.5 void add_constraints_to_surfdata (const Pecos::SurrogateDataVars & *anchor_vars,* const Pecos::SurrogateDataResp & *anchor_resp,* short *fail_code*) [private]

set the anchor point (including gradient and hessian if present) into surf_data

If there is an anchor point, add an equality constraint for its response value. Also add constraints for gradient and hessian, if applicable.

References Dakota::abort_handler(), Dakota::copy_data(), SurfpackApproximation::gradient(), SurfpackApproximation::hessian(), SharedSurfpackApproxData::sdv_to_realarray(), Approximation::sharedDataRep, and SurfpackApproximation::surfData.

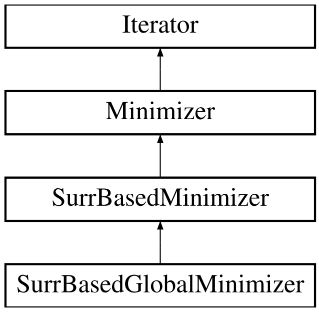
Referenced by SurfpackApproximation::surrogates_to_surf_data().

The documentation for this class was generated from the following files:

- SurfpackApproximation.hpp
- SurfpackApproximation.cpp

14.270 SurrBasedGlobalMinimizer Class Reference

Inheritance diagram for SurrBasedGlobalMinimizer:



Public Member Functions

- SurrBasedGlobalMinimizer (ProblemDescDB &problem_db, Model &model)

    constructor
- ∼SurrBasedGlobalMinimizer ()

    destructor

Protected Member Functions

- void initialize_graphics (int iterator_server_id=1)

    initialize graphics customized for surrogate-based iteration
- void core_run ()

    Performs global surrogate-based optimization by repeatedly optimizing on and improving surrogates of the response functions.
- bool returns_multiple_points () const

    Global surrogate-based methods can return multiple points.

Private Attributes

- bool replacePoints

    flag for replacing the previous iteration's point additions, rather than continuing to append, during construction of the next surrogate

Additional Inherited Members

14.270.1 Detailed Description

This method uses a SurrogateModel to perform minimization (optimization or nonlinear least squares) through a set of iterations. At each iteration, a surrogate is built, the surrogate is minimized, and the optimal points from the surrogate are then evaluated with the "true" function, to generate new points upon which the surrogate for the next iteration is built.

14.270.2 Member Function Documentation

14.270.2.1 void initialize_graphics (int *iterator_server_id* = 1) [inline], [protected], [virtual]

initialize graphics customized for surrogate-based iteration

This just specializes the Iterator implementation to perform default tabulation on the truth model instead of surrogate model.

Reimplemented from Iterator.

References Iterator::initialize_model_graphics(), Iterator::iteratedModel, and Model::truth_model().

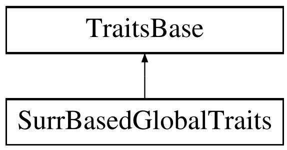
The documentation for this class was generated from the following files:

- SurrBasedGlobalMinimizer.hpp
- SurrBasedGlobalMinimizer.cpp

14.271 SurrBasedGlobalTraits Class Reference

The global surrogate-based minimizer which sequentially minimizes and updates a global surrogate model without trust region controls.

Inheritance diagram for SurrBasedGlobalTraits:



Public Member Functions

- SurrBasedGlobalTraits ()
  default constructor
- virtual ∼SurrBasedGlobalTraits ()
  destructor
- virtual bool is_derived ()
  A temporary query used in the refactor.
- bool supports_continuous_variables ()
  Return the flag indicating whether method supports continuous variables.
- bool supports_discrete_variables ()
  Return the flag indicating whether method supports discrete variables.
- bool supports_linear_equality ()
  Return the flag indicating whether method supports linear equalities.
- bool supports_linear_inequality ()
  Return the flag indicating whether method supports linear inequalities.
- bool supports_nonlinear_equality ()
  Return the flag indicating whether method supports nonlinear equalities.
- bool supports_nonlinear_inequality ()
  Return the flag indicating whether method supports nonlinear inequalities.

14.271.1 Detailed Description

The global surrogate-based minimizer which sequentially minimizes and updates a global surrogate model without trust region controls.

A version of TraitsBase specialized for surrogate-based global minimizer

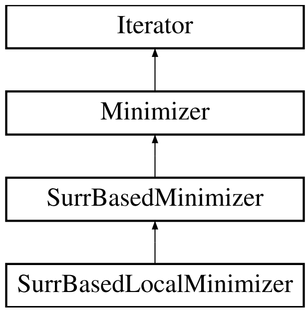
The documentation for this class was generated from the following file:

- SurrBasedGlobalMinimizer.hpp

14.272 SurrBasedLocalMinimizer Class Reference

Class for provably-convergent local surrogate-based optimization and nonlinear least squares.

Inheritance diagram for SurrBasedLocalMinimizer:



Public Member Functions

- SurrBasedLocalMinimizer (ProblemDescDB &problem_db, Model &model, std::shared_ptr< TraitsBase > traits)

  constructor
- SurrBasedLocalMinimizer (Model &model, short merit_fn, short accept_logic, short constr_relax, const RealVector &tr_factors, size_t max_iter, size_t max_eval, Real conv_tol, unsigned short soft_conv_limit, std::shared_ptr< TraitsBase > traits)

  alternate constructor for instantiations "on the fly"
- ∼SurrBasedLocalMinimizer ()

  destructor

Protected Member Functions

- void initialize_graphics (int iterator_server_id=1)

  initialize graphics customized for surrogate-based iteration
- void pre_run ()

  pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori
- void core_run ()

  Performs local surrogate-based minimization by minimizing local, global, or hierarchical surrogates over a series of trust regions.
- void post_run (std::ostream &s)

  post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way
- void reset ()

  restore initial state for repeated sub-iterator executions
- virtual SurrBasedLevelData & trust_region ()=0

  return the active SurrBasedLevelData instance
- virtual void update_trust_region ()=0

  update the trust region bounds, strictly contained within global bounds
- virtual void build ()=0

  build the approximation over the current trust region
- virtual void minimize ()

  solve the approximate subproblem
- virtual void verify ()=0

verify the approximate iterate and update the trust region for the next approximate optimization cycle
- virtual unsigned short converged ()=0

 return the convergence code for the truth level of the trust region hierarchy
- void initialize ()

 shared constructor initializations
- void initialize_sub_model ()

 construct and initialize approxSubProbModel
- void initialize_sub_minimizer ()

 construct and initialize approxSubProbMinimizer
- void initialize_multipliers ()

 initialize lagrangeMult and augLagrangeMult
- void reset_penalties ()

 reset all penalty parameters to their initial values
- void reset_multipliers ()

 reset Lagrange multipliers to initial values for cases where they are accumulated instead of computed directly
- void update_trust_region_data (SurrBasedLevelData &tr_data, const RealVector &parent_l_bnds, const RealVector &parent_u_bnds)

 update the trust region bounds, strictly contained within global bounds
- void update_approx_sub_problem (SurrBasedLevelData &tr_data)

 update variables and bounds within approxSubProbModel
- void compute_trust_region_ratio (SurrBasedLevelData &tr_data, bool check_interior=false)

 compute trust region ratio (for SBLM iterate acceptance and trust region resizing) and check for soft convergence (diminishing returns)
- void hard_convergence_check (SurrBasedLevelData &tr_data, const RealVector &lower_bnds, const RealVector &upper_bnds)

 check for hard convergence (norm of projected gradient of merit function < tolerance)
- void print_convergence_code (std::ostream &s, unsigned short code)

 print out the state corresponding to the code returned by converged()
- void update_penalty (const RealVector &fns_center_truth, const RealVector &fns_star_truth)

 initialize and update the penaltyParameter
- bool find_approx_response (const Variables &search_vars, Response &search_resp)

 locate an approximate response with the data_pairs cache
- bool find_truth_response (const Variables &search_vars, Response &search_resp)

 locate a truth response with the data_pairs cache
- bool find_response (const Variables &search_vars, Response &search_resp, const String &search_id, short set_request)

 locate a response with the data_pairs cache
- void relax_constraints (SurrBasedLevelData &tr_data)

 relax constraints by updating bounds when current iterate is infeasible

Static Protected Member Functions

- static void approx_subprob_objective_eval (const Variables &surrogate_vars, const Variables &recast_vars, const Response &surrogate_response, Response &recast_response)

 static function used to define the approximate subproblem objective.
- static void approx_subprob_constraint_eval (const Variables &surrogate_vars, const Variables &recast_vars, const Response &surrogate_response, Response &recast_response)

 static function used to define the approximate subproblem constraints.
- static void hom_objective_eval (int &mode, int &n, double ∗tau_and_x, double &f, double ∗grad_f, int &)

 static function used by NPSOL as the objective function in the homotopy constraint relaxation formulation.
- static void hom_constraint_eval (int &mode, int &ncnln, int &n, int &nrowj, int ∗needc, double ∗tau_and_x, double ∗c, double ∗cjac, int &nstate)

 static function used by NPSOL as the constraint function in the homotopy constraint relaxation formulation.

Protected Attributes

- Model approxSubProbModel

  the approximate sub-problem formulation solved on each approximate minimization cycle: may be a shallow copy of iteratedModel, or may involve a RecastModel recursion applied to iteratedModel
- short approxSubProbObj

  type of approximate subproblem objective: ORIGINAL_OBJ, LAGRANGIAN_OBJ, or AUGMENTED_LAGRANGIAN-_OBJ
- short approxSubProbCon

  type of approximate subproblem constraints: NO_CON, LINEARIZED_CON, or ORIGINAL_CON
- bool recastSubProb

  flag to indicate when approxSubProbModel involves a RecastModel recursion
- short meritFnType

  type of merit function used in trust region ratio logic: PENALTY_MERIT, ADAPTIVE_PENALTY_MERIT, LAGRANG-IAN_MERIT, or AUGMENTED_LAGRANGIAN_MERIT
- short acceptLogic

  type of iterate acceptance test logic: FILTER or TR_RATIO
- short trConstraintRelax

  type of trust region constraint relaxation for infeasible starting points: NO_RELAX or HOMOTOPY
- int minimizeCycles

  counter for number of minimization cycles that have accumulated prior to convergence at the minimizeIndex level (used for ramping penalties)
- int penaltyIterOffset

  iteration offset used to update the scaling of the penalty parameter for adaptive_penalty merit functions
- RealVector origTrustRegionFactor

  original user specification for trust region initial_size
- Real minTrustRegionFactor

  a soft convergence control: stop SBLM when the trust region factor is reduced below the value of minTrustRegion-Factor
- Real trRatioContractValue

  trust region ratio min value: contract tr if ratio below this value
- Real trRatioExpandValue

  trust region ratio sufficient value: expand tr if ratio above this value
- Real gammaContract

  trust region contraction factor
- Real gammaExpand

  trust region expansion factor
- unsigned short softConvLimit

  convergence control limiting the number of consecutive iterations that fail to achieve sufficient decrease. If exceeded by softConvCount, stop.
- short truthSetRequest

  derivative order of truth data used within the SBLM process
- short approxSetRequest

  derivative order of surrogate data used within the SBLM process
- RealVector initialPoint

  starting point prior to sequence of SBLM iterations
- RealVector globalLowerBnds

  Global lower bounds.
- RealVector globalUpperBnds

  Global Upper bounds.
- RealVector nonlinIneqLowerBndsSlack

  individual violations of nonlinear inequality constraint lower bounds

- RealVector nonlinIneqUpperBndsSlack

  individual violations of nonlinear inequality constraint upper bounds
- RealVector nonlinEqTargetsSlack

  individual violations of nonlinear equality constraint targets
- Real tau

  constraint relaxation parameter
- Real alpha

  constraint relaxation parameter backoff parameter (multiplier)

Static Protected Attributes

- static SurrBasedLocalMinimizer ∗ sblmInstance

  pointer to SBLM instance used in static member functions

Additional Inherited Members

14.272.1 Detailed Description

Class for provably-convergent local surrogate-based optimization and nonlinear least squares.

This minimizer uses a SurrogateModel to perform minimization based on local, global, or hierarchical surrogates. It achieves provable convergence through the use of a sequence of trust regions and the application of surrogate corrections at the trust region centers.

14.272.2 Member Function Documentation

14.272.2.1 void initialize_graphics (int *iterator_server_id* = 1) [protected], [virtual]

initialize graphics customized for surrogate-based iteration

Surrogate-based local (data-fit) specializes graphics to output trust region centers. See OutputManager::add_-tabular_data in DataFitSurrBasedLocalMinimizer. Other children don't do any output

Reimplemented from Iterator.

References Model::create_2d_plots(), Model::create_tabular_datastream(), OutputManager::graph2DFlag, Output-Manager::graphics(), OutputManager::graphics_counter(), Iterator::iteratedModel, Iterator::methodName, Parallel-Library::output_manager(), Iterator::parallelLib, Graphics::set_x_labels2d(), OutputManager::tabular_counter_-label(), OutputManager::tabularDataFlag, and Model::truth_model().

14.272.2.2 void pre_run ( ) [protected], [virtual]

pre-run portion of run (optional); re-implemented by Iterators which can generate all Variables (parameter sets) a priori

pre-run phase, which a derived iterator may optionally reimplement; when not present, pre-run is likely integrated into the derived run function. This is a virtual function; when re-implementing, a derived class must call its nearest parent's pre_run(), if implemented, typically *before* performing its own implementation steps.

Reimplemented from Iterator.

References Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Model::continuous_-variables(), SurrBasedLocalMinimizer::converged(), Dakota::copy_data(), SurrBasedLocalMinimizer::globalLower-Bnds, SurrBasedLocalMinimizer::globalUpperBnds, SurrBasedLocalMinimizer::initialPoint, Iterator::iteratedModel, and SurrBasedLocalMinimizer::reset().

14.272.2.3 void core_run ( ) [protected], [virtual]

Performs local surrogate-based minimization by minimizing local, global, or hierarchical surrogates over a series of trust regions.

Trust region-based strategy to perform surrogate-based optimization in subregions (trust regions) of the parameter space. The minimizer operates on approximations in lieu of the more expensive simulation-based response functions. The size of the trust region is adapted according to the agreement between the approximations and the true response functions.

Reimplemented from Iterator.

References SurrBasedLocalMinimizer::build(), SurrBasedLocalMinimizer::converged(), SurrBasedLocalMinimizer::minimize(), SurrBasedLocalMinimizer::sblmInstance, SurrBasedLocalMinimizer::update_trust_region(), and SurrBasedLocalMinimizer::verify().

14.272.2.4 void post_run (std::ostream & *s*) [protected], [virtual]

post-run portion of run (optional); verbose to print results; re-implemented by Iterators that can read all Variables/Responses and perform final analysis phase in a standalone way

Post-run phase, which a derived iterator may optionally reimplement; when not present, post-run is likely integrated into run. This is a virtual function; when re-implementing, a derived class must call its nearest parent's post_run(), typically *after* performing its own implementation steps.

Reimplemented from Minimizer.

References SurrBasedLocalMinimizer::converged(), SurrBasedMinimizer::globalIterCount, Minimizer::post_run(), and SurrBasedLocalMinimizer::print_convergence_code().

14.272.2.5 void compute_trust_region_ratio (SurrBasedLevelData & *tr_data*, bool *check_interior* = false) [protected]

compute trust region ratio (for SBLM iterate acceptance and trust region resizing) and check for soft convergence (diminishing returns)

Assess acceptance of SBLM iterate (trust region ratio or filter) and compute soft convergence metrics (number of consecutive failures, min trust region size, etc.) to assess whether the convergence rate has decreased to a point where the process should be terminated (diminishing returns).

References SurrBasedLocalMinimizer::acceptLogic, SurrBasedLocalMinimizer::approxSubProbObj, SurrBasedMinimizer::augmented_lagrangian_merit(), SurrBasedMinimizer::constraint_violation(), Minimizer::constraintTol, Iterator::convergenceTol, SurrBasedMinimizer::etaSequence, Response::function_values(), SurrBasedLocalMinimizer::gammaContract, SurrBasedLocalMinimizer::gammaExpand, SurrBasedLocalMinimizer::globalLowerBnds, SurrBasedLocalMinimizer::globalUpperBnds, SurrBasedMinimizer::initialize_filter(), Response::is_null(), Iterator::iteratedModel, SurrBasedMinimizer::lagrangian_merit(), SurrBasedLocalMinimizer::meritFnType, Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, Minimizer::objective(), SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, Iterator::outputLevel, SurrBasedMinimizer::penalty_merit(), Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), Response::reset(), SurrBasedLocalMinimizer::softConvLimit, SurrBasedLocalMinimizer::trRatioContractValue, SurrBasedLocalMinimizer::trRatioExpandValue, SurrBasedMinimizer::update_augmented_lagrange_multipliers(), SurrBasedMinimizer::update_filter(), and SurrBasedLocalMinimizer::update_penalty().

14.272.2.6 void hard_convergence_check (SurrBasedLevelData & *tr_data*, const RealVector & *lower_bnds*, const RealVector & *upper_bnds*) [protected]

check for hard convergence (norm of projected gradient of merit function $<$ tolerance)

The hard convergence check computes the gradient of the merit function at the trust region center, performs a projection for active bound constraints (removing any gradient component directed into an active bound), and signals convergence if the 2-norm of this projected gradient is less than convergenceTol.

References SurrBasedLocalMinimizer::approxSubProbObj, SurrBasedMinimizer::constraint_violation(), Minimizer::constraintTol, Iterator::convergenceTol, Response::function_gradients(), Response::function_values(), Iterator::iteratedModel, SurrBasedMinimizer::lagrangian_gradient(), SurrBasedLocalMinimizer::meritFnType, SurrBasedLocalMinimizer::minimizeCycles, Minimizer::numContinuousVars, Minimizer::numNonlinearConstraints, SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, Iterator::outputLevel, Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), SurrBasedLocalMinimizer::truthSetRequest, SurrBasedMinimizer::update_augmented_lagrange_multipliers(), and SurrBasedMinimizer::update_lagrange_multipliers().

14.272.2.7 void update_penalty (const RealVector & *fns_center_truth*, const RealVector & *fns_star_truth*) [protected]

initialize and update the penaltyParameter

Scaling of the penalty value is important to avoid rejecting SBLM iterates which must increase the objective to achieve a reduction in constraint violation. In the basic penalty case, the penalty is ramped exponentially based on the iteration counter. In the adaptive case, the ratio of relative change between center and star points for the objective and constraint violation values is used to rescale penalty values.

References SurrBasedMinimizer::alphaEta, SurrBasedLocalMinimizer::approxSubProbObj, SurrBasedMinimizer::constraint_violation(), Minimizer::constraintTol, SurrBasedMinimizer::eta, SurrBasedMinimizer::etaSequence, Iterator::iteratedModel, SurrBasedLocalMinimizer::meritFnType, SurrBasedLocalMinimizer::minimizeCycles, Minimizer::objective(), Iterator::outputLevel, SurrBasedLocalMinimizer::penaltyIterOffset, SurrBasedMinimizer::penaltyParameter, Model::primary_response_fn_sense(), and Model::primary_response_fn_weights().

Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio().

14.272.2.8 void approx_subprob_objective_eval (const Variables & *surrogate_vars*, const Variables & *recast_vars*, const Response & *surrogate_response*, Response & *recast_response*) [static], [protected]

static function used to define the approximate subproblem objective.

Objective functions evaluator for solution of approximate subproblem using a RecastModel.

References Response::active_set_request_vector(), SurrBasedLocalMinimizer::approxSubProbCon, SurrBasedLocalMinimizer::approxSubProbModel, SurrBasedLocalMinimizer::approxSubProbObj, SurrBasedMinimizer::augmented_lagrangian_gradient(), SurrBasedMinimizer::augmented_lagrangian_hessian(), SurrBasedMinimizer::augmented_lagrangian_merit(), Response::function_gradient(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian(), Response::function_hessians(), Response::function_value(), Response::function_values(), Iterator::iteratedModel, SurrBasedMinimizer::lagrangian_gradient(), SurrBasedMinimizer::lagrangian_hessian(), SurrBasedMinimizer::lagrangian_merit(), Model::nonlinear_eq_constraint_targets(), Model::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Minimizer::numUserPrimaryFns, Minimizer::objective(), Minimizer::objective_gradient(), Minimizer::objective_hessian(), SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, Model::primary_response_fn_sense(), Model::primary_response_fn_weights(), and SurrBasedLocalMinimizer::sblmInstance.

Referenced by SurrBasedLocalMinimizer::initialize_sub_model().

14.272.2.9 void approx_subprob_constraint_eval (const Variables & *surrogate_vars*, const Variables & *recast_vars*, const Response & *surrogate_response*, Response & *recast_response*) [static], [protected]

static function used to define the approximate subproblem constraints.

Constraint functions evaluator for solution of approximate subproblem using a RecastModel.

References Response::active_set_derivative_vector(), Response::active_set_request_vector(), SurrBasedLocalMinimizer::approxSubProbCon, SurrBasedLocalMinimizer::approxSubProbObj, Variables::continuous_variables(), Response::function_gradient(), Response::function_gradient_view(), Response::function_gradients(), Response::function_hessian(), Response::function_hessian_view(), Response::function_value(), Response::function_-

values(), Minimizer::numUserPrimaryFns, SurrBasedLocalMinimizer::sblmInstance, and SurrBasedLocalMinimizer-::trust_region().

Referenced by SurrBasedLocalMinimizer::initialize_sub_model().

14.272.2.10 void hom_objective_eval (int & *mode,* int & *n,* double ∗ *tau_and_x,* double & *f,* double ∗ *grad_f,* int &) [static], [protected]

static function used by NPSOL as the objective function in the homotopy constraint relaxation formulation.

NPSOL objective functions evaluator for solution of homotopy constraint relaxation parameter optimization. This constrained optimization problem performs the update of the tau parameter in the homotopy heuristic approach used to relax the constraints in the original problem .

Referenced by SurrBasedLocalMinimizer::relax_constraints().

14.272.2.11 void hom_constraint_eval (int & *mode,* int & *ncnln,* int & *n,* int & *nrowj,* int ∗ *needc,* double ∗ *tau_and_x,* double ∗ *c,* double ∗ *cjac,* int & *nstate*) [static], [protected]

static function used by NPSOL as the constraint function in the homotopy constraint relaxation formulation.

NPSOL constraint functions evaluator for solution of homotopy constraint relaxation parameter optimization. This constrained optimization problem performs the update of the tau parameter in the homotopy heuristic approach used to relax the constraints in the original problem.

References Response::active_set(), SurrBasedLocalMinimizer::approxSubProbModel, Model::continuous_-variables(), Model::current_response(), Model::evaluate(), Response::function_gradients(), Response::function_-values(), SurrBasedLocalMinimizer::nonlinEqTargetsSlack, SurrBasedLocalMinimizer::nonlinIneqLowerBndsSlack, SurrBasedLocalMinimizer::nonlinIneqUpperBndsSlack, Minimizer::numNonlinearEqConstraints, Minimizer::num-NonlinearIneqConstraints, ActiveSet::request_vector(), Model::response_size(), SurrBasedLocalMinimizer::sblm-Instance, and SurrBasedLocalMinimizer::tau.

Referenced by SurrBasedLocalMinimizer::relax_constraints().

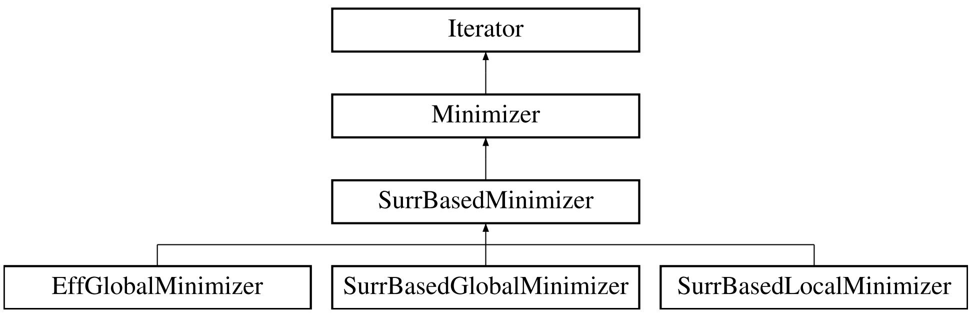
The documentation for this class was generated from the following files:

- SurrBasedLocalMinimizer.hpp
- SurrBasedLocalMinimizer.cpp

14.273 SurrBasedMinimizer Class Reference

Base class for local/global surrogate-based optimization/least squares.

Inheritance diagram for SurrBasedMinimizer:



Protected Member Functions

- SurrBasedMinimizer (ProblemDescDB &problem_db, Model &model, std::shared_ptr< TraitsBase > traits)

  constructor
- SurrBasedMinimizer (Model &model, size_t max_iter, size_t max_eval, Real conv_tol, std::shared_ptr< TraitsBase > traits)

  alternate constructor for instantiations "on the fly"
- ∼SurrBasedMinimizer ()

  destructor
- void derived_init_communicators (ParLevLIter pl_iter)

  derived class contributions to initializing the communicators associated with this Iterator instance
- void derived_set_communicators (ParLevLIter pl_iter)

  derived class contributions to setting the communicators associated with this Iterator instance
- void derived_free_communicators (ParLevLIter pl_iter)

  derived class contributions to freeing the communicators associated with this Iterator instance
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)
- void initialize_from_model (Model &model)

  helper for shared ctor code
- void update_lagrange_multipliers (const RealVector &fn_vals, const RealMatrix &fn_grads, SurrBasedLevelData &tr_data)

  initialize and update Lagrange multipliers for basic Lagrangian
- void update_augmented_lagrange_multipliers (const RealVector &fn_vals)

  initialize and update the Lagrange multipliers for augmented Lagrangian
- void initialize_filter (SurrBasedLevelData &tr_data, const RealVector &fn_vals)

  (re-)initialize filter from a set of function values
- bool update_filter (SurrBasedLevelData &tr_data, const RealVector &fn_vals)

  update filter using a new set of function values
- Real lagrangian_merit (const RealVector &fn_vals, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts)

  compute a Lagrangian function from a set of function values
- void lagrangian_gradient (const RealVector &fn_vals, const RealMatrix &fn_grads, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, RealVector &lag_grad)

  compute the gradient of the Lagrangian function
- void lagrangian_hessian (const RealVector &fn_vals, const RealMatrix &fn_grads, const RealSymMatrixArray &fn_hessians, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, RealSymMatrix &lag_hess)

  compute the Hessian of the Lagrangian function
- Real augmented_lagrangian_merit (const RealVector &fn_vals, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts)

  compute an augmented Lagrangian function from a set of function values
- void augmented_lagrangian_gradient (const RealVector &fn_vals, const RealMatrix &fn_grads, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, RealVector &alag_grad)

  compute the gradient of the augmented Lagrangian function
- void augmented_lagrangian_hessian (const RealVector &fn_vals, const RealMatrix &fn_grads, const RealSymMatrixArray &fn_hessians, const BoolDeque &sense, const RealVector &primary_wts, const RealVector &nln_ineq_l_bnds, const RealVector &nln_ineq_u_bnds, const RealVector &nln_eq_tgts, RealSymMatrix &alag_hess)

  compute the Hessian of the augmented Lagrangian function
- Real penalty_merit (const RealVector &fn_vals, const BoolDeque &sense, const RealVector &primary_wts)

compute a penalty function from a set of function values

- void penalty_gradient (const RealVector &fn_vals, const RealMatrix &fn_grads, const BoolDeque &sense, const RealVector &primary_wts, RealVector &pen_grad)

  compute the gradient of the penalty function
- Real constraint_violation (const RealVector &fn_vals, const Real &constraint_tol)

  compute the constraint violation from a set of function values

Protected Attributes

- Iterator approxSubProbMinimizer

  the minimizer used on the surrogate model to solve the approximate subproblem on each surrogate-based iteration
- size_t globalIterCount

  global iteration counter corresponding to number of surrogate-based minimizations
- RealVector lagrangeMult

  Lagrange multipliers for basic Lagrangian calculations.
- RealVector augLagrangeMult

  Lagrange multipliers for augmented Lagrangian calculations.
- Real penaltyParameter

  the penalization factor for violated constraints used in quadratic penalty calculations; increased in update_penalty()
- RealVector origNonlinIneqLowerBnds

  original nonlinear inequality constraint lower bounds (no relaxation)
- RealVector origNonlinIneqUpperBnds

  original nonlinear inequality constraint upper bounds (no relaxation)
- RealVector origNonlinEqTargets

  original nonlinear equality constraint targets (no relaxation)
- Real eta

  constant used in etaSequence updates
- Real alphaEta

  power for etaSequence updates when updating penalty
- Real betaEta

  power for etaSequence updates when updating multipliers
- Real etaSequence

  decreasing sequence of allowable constraint violation used in augmented Lagrangian updates (refer to Conn, Gould, and Toint, section 14.4)
- size_t miPLIndex

  index for the active ParallelLevel within ParallelConfiguration::miPLIters

Additional Inherited Members

14.273.1 Detailed Description

Base class for local/global surrogate-based optimization/least squares.

These minimizers use a SurrogateModel to perform optimization based either on local trust region methods or global updating methods.

14.273.2 Member Function Documentation

14.273.2.1 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

Redefines default iterator results printing to include optimization results (objective functions and constraints).

Reimplemented from Iterator.

References Dakota::abort_handler(), Iterator::activeSet, Iterator::bestResponseArray, Iterator::bestVariablesArray, Model::interface_id(), Iterator::iteratedModel, Iterator::methodName, Minimizer::numFunctions, Minimizer::numUserPrimaryFns, Minimizer::optimizationFlag, Minimizer::print_best_eval_ids(), Minimizer::print_residuals(), ActiveSet::request_values(), and Model::truth_model().

14.273.2.2 void update_lagrange_multipliers (const RealVector & *fn_vals*, const RealMatrix & *fn_grads*, SurrBasedLevelData & *tr_data*) [protected]

initialize and update Lagrange multipliers for basic Lagrangian

For the Rockafellar augmented Lagrangian, simple Lagrange multiplier updates are available which do not require the active constraint gradients. For the basic Lagrangian, Lagrange multipliers are estimated through solution of a nonnegative linear least squares problem.

References Dakota::abort_handler(), Minimizer::bigRealBoundSize, Minimizer::constraintTol, Model::continuous_lower_bounds(), Model::continuous_upper_bounds(), Iterator::iteratedModel, SurrBasedMinimizer::lagrangeMult, Minimizer::numContinuousVars, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, Minimizer::objective_gradient(), SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, Model::primary_response_fn_sense(), and Model::primary_response_fn_weights().

Referenced by SurrBasedLocalMinimizer::hard_convergence_check().

14.273.2.3 void update_augmented_lagrange_multipliers (const RealVector & *fn_vals*) [protected]

initialize and update the Lagrange multipliers for augmented Lagrangian

For the Rockafellar augmented Lagrangian, simple Lagrange multiplier updates are available which do not require the active constraint gradients. For the basic Lagrangian, Lagrange multipliers are estimated through solution of a nonnegative linear least squares problem.

References SurrBasedMinimizer::augLagrangeMult, SurrBasedMinimizer::betaEta, Minimizer::bigRealBoundSize, SurrBasedMinimizer::etaSequence, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, SurrBasedMinimizer::origNonlinIneqUpperBnds, and SurrBasedMinimizer::penaltyParameter.

Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio(), SurrBasedLocalMinimizer::hard_convergence_check(), and EffGlobalMinimizer::update_constraints().

14.273.2.4 bool update_filter (SurrBasedLevelData & *tr_data*, const RealVector & *fn_vals*) [protected]

update filter using a new set of function values

Update the paretoFilter with fn_vals if new iterate is non-dominated.

References SurrBasedMinimizer::constraint_violation(), Iterator::iteratedModel, Minimizer::numNonlinearConstraints, Minimizer::objective(), Model::primary_response_fn_sense(), and Model::primary_response_fn_weights().

Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio().

14.273.2.5 Real lagrangian_merit (const RealVector & *fn_vals,* const BoolDeque & *sense,* const RealVector & *primary_wts,* const RealVector & *nln_ineq_l_bnds,* const RealVector & *nln_ineq_u_bnds,* const RealVector & *nln_eq_tgts*) [protected]

compute a Lagrangian function from a set of function values

The Lagrangian function computation sums the objective function and the Lagrange multipler terms for inequality/equality constraints. This implementation follows the convention in Vanderplaats with g<=0 and h=0. The bounds/targets passed in may reflect the original constraints or the relaxed constraints.

References Minimizer::bigRealBoundSize, Minimizer::constraintTol, SurrBasedMinimizer::lagrangeMult, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, and Minimizer::objective().

Referenced by SurrBasedLocalMinimizer::approx_subprob_objective_eval(), and SurrBasedLocalMinimizer::compute_trust_region_ratio().

14.273.2.6 Real augmented_lagrangian_merit (const RealVector & *fn_vals,* const BoolDeque & *sense,* const RealVector & *primary_wts,* const RealVector & *nln_ineq_l_bnds,* const RealVector & *nln_ineq_u_bnds,* const RealVector & *nln_eq_tgts*) [protected]

compute an augmented Lagrangian function from a set of function values

The Rockafellar augmented Lagrangian function sums the objective function, Lagrange multipler terms for inequality/equality constraints, and quadratic penalty terms for inequality/equality constraints. This implementation follows the convention in Vanderplaats with g<=0 and h=0. The bounds/targets passed in may reflect the original constraints or the relaxed constraints.

References SurrBasedMinimizer::augLagrangeMult, Minimizer::bigRealBoundSize, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, Minimizer::objective(), and SurrBasedMinimizer::penaltyParameter.

Referenced by SurrBasedLocalMinimizer::approx_subprob_objective_eval(), EffGlobalMinimizer::augmented_lagrangian(), and SurrBasedLocalMinimizer::compute_trust_region_ratio().

14.273.2.7 Real penalty_merit (const RealVector & *fn_vals,* const BoolDeque & *sense,* const RealVector & *primary_wts*) [protected]

compute a penalty function from a set of function values

The penalty function computation applies a quadratic penalty to any constraint violations and adds this to the objective function(s) p = f + r_p cv.

References SurrBasedMinimizer::constraint_violation(), Minimizer::constraintTol, Minimizer::objective(), and SurrBasedMinimizer::penaltyParameter.

Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio().

14.273.2.8 Real constraint_violation (const RealVector & *fn_vals,* const Real & *constraint_tol*) [protected]

compute the constraint violation from a set of function values

Compute the quadratic constraint violation defined as cv = g+^T g+

- h+^T h+. This implementation supports equality constraints and 2-sided inequalities. The constraint_tol allows for a small constraint infeasibility (used for penalty methods, but not Lagrangian methods).

References Minimizer::bigRealBoundSize, Minimizer::numNonlinearEqConstraints, Minimizer::numNonlinearIneqConstraints, Minimizer::numUserPrimaryFns, SurrBasedMinimizer::origNonlinEqTargets, SurrBasedMinimizer::origNonlinIneqLowerBnds, and SurrBasedMinimizer::origNonlinIneqUpperBnds.

Referenced by SurrBasedLocalMinimizer::compute_trust_region_ratio(), SurrBasedLocalMinimizer::hard_-convergence_check(), SurrBasedMinimizer::initialize_filter(), SurrBasedMinimizer::penalty_merit(), SurrBased-LocalMinimizer::relax_constraints(), EffGlobalMinimizer::update_constraints(), SurrBasedMinimizer::update_filter(), and SurrBasedLocalMinimizer::update_penalty().

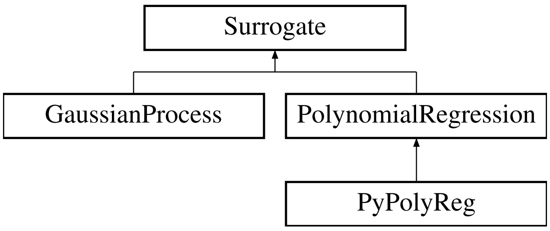
The documentation for this class was generated from the following files:

- SurrBasedMinimizer.hpp
- SurrBasedMinimizer.cpp

14.274 Surrogate Class Reference

Parent class for surrogate models.

Inheritance diagram for Surrogate:



Public Member Functions

- Surrogate ()

  Constructor that uses defaultConfigOptions and does not build.
- Surrogate (const ParameterList &param_list)

  Constructor that sets configOptions but does not build.
- Surrogate (const MatrixXd &samples, const MatrixXd &response, const ParameterList &param_list)

  Constructor for the Surrogate that sets configOptions and builds the surrogate (does nothing in the base class).
- virtual ∼Surrogate ()

  Default destructor.
- virtual void build (const MatrixXd &samples, const MatrixXd &response)=0

  Build the Surrogate using specified build data.
- virtual VectorXd value (const MatrixXd &eval_points, const int qoi)=0

  Evaluate the Surrogate at a set of prediction points for a single QoI.
- VectorXd value (const MatrixXd &eval_points)

  Evaluate the Surrogate at a set of prediction points for QoI index 0.
- virtual MatrixXd gradient (const MatrixXd &eval_points, const int qoi)

  Evaluate the gradient of the Surrogate at a set of prediction points.
- MatrixXd gradient (const MatrixXd &eval_points)

  Evaluate the gradient of the Surrogate at a set of prediction points for QoI index 0.
- virtual MatrixXd hessian (const MatrixXd &eval_point, const int qoi)

  Evaluate the Hessian of the Surrogate at a single point.
- MatrixXd hessian (const MatrixXd &eval_point)

  Evaluate the Hessian of the Surrogate at a single point for QoI index 0.
- void variable_labels (const std::vector< std::string > &var_labels)

  Set the variable/feature names.
- const std::vector< std::string > & variable_labels () const

  Get the (possibly empty) variable/feature names.

- void response_labels (const std::vector< std::string > &resp_labels)

  Set the response/QoI names.
- const std::vector< std::string > & response_labels () const

  Get the (possibly empty) response/QoI names.
- void set_options (const ParameterList &options)

  Set the Surrogate's configOptions.
- void get_options (ParameterList &options)

  Get the Surrogate's configOptions.
- void print_options ()

  Print the Surrogate's configOptions.
- virtual void default_options ()=0

  Initialize the Surrogate's defaultConfigOptions.
- VectorXd evaluate_metrics (const StringArray &mnames, const MatrixXd &points, const MatrixXd &ref_-values)

  Evalute metrics at specified points (within surrogates)
- VectorXd cross_validate (const MatrixXd &samples, const MatrixXd &response, const StringArray &mnames, const int num_folds=5, const int seed=20)

  Perform K-folds cross-validation (within surrogates)
- template<typename DerivedSurr >
  void save (const DerivedSurr &surr_out, const std::string &outfile, const bool binary)

  Serialize a derived (i.e. non-base) surrogate model.
- template<typename DerivedSurr >
  void load (const std::string &infile, const bool binary, DerivedSurr &surr_in)

  Load a derived (i.e. non-base) surrogate model.

Static Public Member Functions

- template<typename SurrHandle >
  static void save (const SurrHandle &surr_out, const std::string &outfile, const bool binary)

  serialize Surrogate to file (typically through shared_ptr<Surrogate>, but Derived& or Derived okay too)*
- template<typename SurrHandle >
  static void load (const std::string &infile, const bool binary, SurrHandle &surr_in)

  serialize Surrogate from file (typically through shared_ptr<Surrogate>, but Derived& or Derived okay too)*
- static std::shared_ptr< Surrogate > load (const std::string &infile, const bool binary)

  serialize Surrogate from file through pointer to base class (must have been saved via same data type)

Public Attributes

- util::DataScaler dataScaler

  DataScaler class for a Surrogate's build samples.
- double responseOffset = 0.

  Response offset.
- double responseScaleFactor = 1.

  Response scale factor.

Protected Member Functions

- virtual std::shared_ptr
  < Surrogate > clone () const =0

  clone derived Surrogate class for use in cross-validation

Protected Attributes

- int numSamples

  Number of samples in the Surrogate's build samples.
- int numVariables

  Number of features/variables in the Surrogate's build samples.
- std::vector< std::string > variableLabels

  Names of the variables/features; need not be populated.
- int numQOI

  Number of quantities of interest predicted by the surrogate. For scalar-valued surrogates numQOI = 1.
- std::vector< std::string > responseLabels

  Names of the responses/QoIs; need not be populated.
- ParameterList defaultConfigOptions

  Default Key/value options to configure the surrogate.
- ParameterList configOptions

  Key/value options to configure the surrogate - will override defaultConfigOptions.

Private Member Functions

- template<class Archive >
  void serialize (Archive &archive, const unsigned int version)

  Serializer for base class data (call from dervied with base_object)

Friends

- class boost::serialization::access

  Allow serializers access to private class data.

14.274.1 Detailed Description

Parent class for surrogate models.

The Surrogate class defines the API for surrogate models contained in the Dakota surrogates module.

Pure virtual functions include build, value, and default_options. Gradient and Hessian methods are optional.

Configuration options for a surrogate are set through the use of a Teuchos ParameterList named configOptions.

14.274.2 Constructor & Destructor Documentation

14.274.2.1 Surrogate (const ParameterList & *param_list*)

Constructor that sets configOptions but does not build.

Parameters

in	*param_list*	List that overrides entries in defaultConfigOptions.

References Surrogate::numQOI, and dakota::silence_unused_args().

14.274.2.2 Surrogate (const MatrixXd & *samples*, const MatrixXd & *response*, const ParameterList & *param_list*)

Constructor for the Surrogate that sets configOptions and builds the surrogate (does nothing in the base class).

Parameters

in	*samples*	Matrix of data for surrogate construction - (num_samples by num_features).
in	*response*	Vector of targets for surrogate construction - (num_samples by num_qoi = 1; only 1 response is supported currently).
in	*param_list*	List that overrides entries in defaultConfigOptions.

References Surrogate::numQOI, and dakota::silence_unused_args().

14.274.3 Member Function Documentation

14.274.3.1 virtual void build (const MatrixXd & *samples*, const MatrixXd & *response*) [pure virtual]

Build the Surrogate using specified build data.

Parameters

in	*samples*	Matrix of data for surrogate construction - (num_samples by num_features).
in	*response*	Vector of responses/targets for surrogate construction - (num_samples by num_qoi = 1).

Implemented in GaussianProcess, and PolynomialRegression.

14.274.3.2 virtual VectorXd value (const MatrixXd & *eval_points*, const int *qoi*) [pure virtual]

Evaluate the Surrogate at a set of prediction points for a single QoI.

Parameters

in	*eval_points*	Matrix of prediction points - (num_pts by num_features).
in	*qoi*	Index for surrogate QoI.

Returns

Values of the Surrogate at the prediction points - (num_pts).

Implemented in GaussianProcess, and PolynomialRegression.

Referenced by Surrogate::evaluate_metrics(), dakota::surrogates::fd_check_gradient(), dakota::surrogates::fd-_check_hessian(), PYBIND11_MODULE(), PyPolyReg::value(), PolynomialRegression::value(), and Gaussian-Process::value().

14.274.3.3 VectorXd value (const MatrixXd & *eval_points*) [inline]

Evaluate the Surrogate at a set of prediction points for QoI index 0.

Parameters

in	*eval_points*	Vector of prediction points - (num_features).

Returns

Values of the Surrogate at the prediction points - (num_pts).

References Surrogate::value().

Referenced by Surrogate::value().

14.274.3.4 MatrixXd gradient (const MatrixXd & *eval_points*, const int *qoi*) [virtual]

Evaluate the gradient of the Surrogate at a set of prediction points.

Parameters

in	*eval_points*	Matrix of prediction points - (num_pts by num_features).
in	*qoi*	Index of the quantity of interest for gradient evaluation - 0 for scalar-valued surrogates.

Returns

Matrix of gradient vectors at the prediction points - (num_pts by num_features).

Reimplemented in GaussianProcess, and PolynomialRegression.

References dakota::silence_unused_args().

Referenced by dakota::surrogates::fd_check_gradient(), Surrogate::gradient(), PolynomialRegression::gradient(), GaussianProcess::gradient(), and PYBIND11_MODULE().

14.274.3.5 MatrixXd gradient (const MatrixXd & *eval_points*) [inline]

Evaluate the gradient of the Surrogate at a set of prediction points for QoI index 0.

Parameters

in	*eval_points*	Matrix of prediction points • (num_pts by num_features).

Returns

Matrix of gradient vectors at the prediction points - (num_pts by num_features).

References Surrogate::gradient().

14.274.3.6 MatrixXd hessian (const MatrixXd & *eval_point,* const int *qoi*) [virtual]

Evaluate the Hessian of the Surrogate at a single point.

Parameters

in	*eval_point*	Coordinates of the prediction point - (1 by num_features).
in	*qoi*	Index of the quantity of interest for Hessian evaluation - 0 for scalar-valued surrogates.

Returns

Hessian matrix at the prediction point - (num_features by num_features).

Reimplemented in GaussianProcess, and PolynomialRegression.

References dakota::silence_unused_args().

Referenced by dakota::surrogates::fd_check_hessian(), Surrogate::hessian(), GaussianProcess::hessian(), PolynomialRegression::hessian(), and PYBIND11_MODULE().

14.274.3.7 MatrixXd hessian (const MatrixXd & *eval_point*) [inline]

Evaluate the Hessian of the Surrogate at a single point for QoI index 0.

Parameters

in	*eval_point*	Coordinates of the prediction point - (1 by num_features).

Returns

Hessian matrix at the prediction point - (num_features by num_features).

References Surrogate::hessian().

14.274.3.8 void variable_labels (const std::vector< std::string > & *var_labels*)

Set the variable/feature names.

Parameters

in	*var_labels*	Vector of strings, one per input variable

References Surrogate::variableLabels.

14.274.3.9 const std::vector< std::string > & variable_labels ( ) const

Get the (possibly empty) variable/feature names.

Returns

Vector of strings, one per input variable; empty if not set

References Surrogate::variableLabels.

Referenced by PYBIND11_MODULE().

14.274.3.10 void response_labels (const std::vector< std::string > & *resp_labels*)

Set the response/QoI names.

Parameters

in	*resp_labels*	Vector of strings, one per surrogate response

References Surrogate::responseLabels.

14.274.3.11 const std::vector< std::string > & response_labels ( ) const

Get the (possibly empty) response/QoI names.

Returns

Vector of strings, one per surrogate response; empty if not set

References Surrogate::responseLabels.

Referenced by PYBIND11_MODULE().

14.274.3.12 void set_options (const **ParameterList** & *options*)

Set the Surrogate's configOptions.

Parameters

in	*options*	ParameterList of configuration options.

References Surrogate::configOptions.

14.274.3.13 void get_options (ParameterList & *options*)

Get the Surrogate's configOptions.

Parameters

out	*options*	ParameterList of configuration options.

References Surrogate::configOptions.

14.274.3.14 void save (const DerivedSurr & *surr_out*, const std::string & *outfile*, const bool *binary*)

Serialize a derived (i.e. non-base) surrogate model.

Parameters

in	*surr_out*	Surrogate to seralize.
in	*outfile*	Name of the output text or binary file.
in	*binary*	Flag for binary or text format.

14.274.3.15 void load (const std::string & *infile*, const bool *binary*, DerivedSurr & *surr_in*)

Load a derived (i.e. non-base) surrogate model.

Parameters

in	*infile*	Filename for serialized surrogate.
in	*binary*	Flag for binary or text format.
in	*surr_in*	Derived surrogate class to be populated with serialized data.

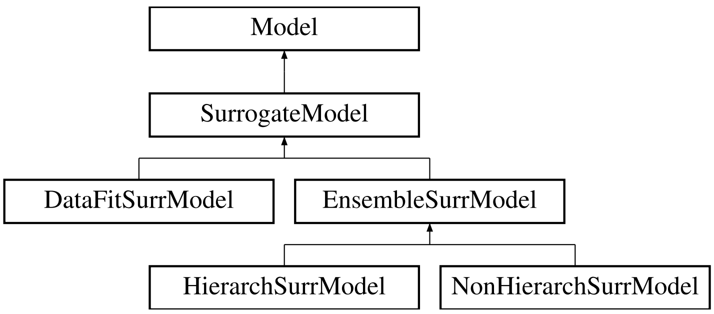
The documentation for this class was generated from the following files:

- SurrogatesBase.hpp
- SurrogatesBase.cpp

14.275 SurrogateModel Class Reference

Base class for surrogate models (DataFitSurrModel and HierarchSurrModel).

Inheritance diagram for SurrogateModel:



Protected Member Functions

- SurrogateModel (ProblemDescDB &problem_db)

  constructor
- SurrogateModel (ProblemDescDB &problem_db, ParallelLibrary &parallel_lib, const SharedVariablesData &svd, bool share_svd, const SharedResponseData &srd, bool share_srd, const ActiveSet &set, short corr_-type, short output_level)

  alternate constructor
- ∼SurrogateModel ()

  destructor
- Pecos::ProbabilityTransformation & probability_transformation ()

  return probability transformation employed by the Model (forwarded along to ProbabilityTransformModel recasting)
- void activate_distribution_parameter_derivatives ()

  activate derivative setting w.r.t. distribution parameters
- void deactivate_distribution_parameter_derivatives ()

  deactivate derivative setting w.r.t. distribution parameters
- void trans_grad_X_to_U (const RealVector &fn_grad_x, RealVector &fn_grad_u, const RealVector &x_vars)

  transform x-space gradient vector to u-space
- void trans_grad_U_to_X (const RealVector &fn_grad_u, RealVector &fn_grad_x, const RealVector &x_vars)

  transform u-space gradient vector to x-space
- void trans_grad_X_to_S (const RealVector &fn_grad_x, RealVector &fn_grad_s, const RealVector &x_vars)

  transform x-space gradient vector to gradient with respect to inserted distribution parameters
- void trans_hess_X_to_U (const RealSymMatrix &fn_hess_x, RealSymMatrix &fn_hess_u, const RealVector &x_vars, const RealVector &fn_grad_x)

  transform x-space Hessian matrix to u-space
- Model & subordinate_model ()

  return truth_model()
- void active_model_key (const Pecos::ActiveKey &key)

  set the active model key within surrogate data, grid driver, and approximation classes that support the management of multiple approximation states within surrogate models
- const Pecos::ActiveKey & active_model_key () const

  return the active model key (used by surrogate data, grid driver, and approximation classes to support the management of multiple approximation states within surrogate models)
- short surrogate_response_mode () const

  return responseMode
- int derived_evaluation_id () const

  return the current evaluation id for this Model
- size_t mi_parallel_level_index () const

  return miPLIndex
- virtual void check_submodel_compatibility (const Model &sub_model)=0

  verify compatibility between SurrogateModel attributes and attributes of the submodel (DataFitSurrModel::actualModel or HierarchSurrModel::highFidelityModel)
- virtual void init_model (Model &model)

  initialize model with data that could change once per set of evaluations (e.g., an outer iterator execution), including active variable labels, inactive variable values/bounds/labels, and linear/nonlinear constraint coeffs/bounds
- virtual void update_model (Model &model)

  update model with data that could change per function evaluation (active variable values/bounds)
- virtual void update_from_model (const Model &model)

  update current variables/labels/bounds/targets with data from model
- virtual size_t insert_response_start (size_t position)

  compute start index for inserting response data into aggregated response
- virtual void insert_metadata (const RealArray &md, size_t position, Response &agg_response)

insert a single response into an aggregated response in the specified position

- bool check_active_variables (const Model &sub_model)

  check sub_model for consistency in active variable counts

- bool check_inactive_variables (const Model &sub_model)

  check sub_model for consistency in inactive variable counts

- bool check_response_qoi (const Model &sub_model)

  check sub_model for consistency in response QoI counts

- void asv_split (const ShortArray &orig_asv, ShortArray &actual_asv, ShortArray &approx_asv, bool build_flag)

  distributes the incoming orig_asv among actual_asv and approx_asv

- void asv_split (const ShortArray &orig_asv, Short2DArray &indiv_asv)

  distributes the incoming orig_asv among actual_asv and approx_asv

- void init_model_constraints (Model &model)

  initialize model with linear/nonlinear constraint data that could change once per set of evaluations (e.g., an outer iterator execution)

- void init_model_labels (Model &model)

  initialize model with active/inactive variable label data that could change once per set of evaluations (e.g., an outer iterator execution)

- void init_model_inactive_variables (Model &model)

  initialize model with inactive variable values/bounds data that could change once per set of evaluations (e.g., an outer iterator execution)

- void init_model_inactive_labels (Model &model)

  initialize model with inactive variable labels that could change once per set of evaluations (e.g., an outer iterator execution)

- void update_model_active_variables (Model &model)

  update model with active variable values/bounds data

- void update_model_distributions (Model &model)

  update model with random variable distribution data

- void update_variables_from_model (const Model &model)

  update current variables/bounds with data from model

- void update_distributions_from_model (const Model &model)

  update current random variable distributions with data from model

- void update_response_from_model (const Model &model)

  update response/constraints with data from model

- void check_key (int key1, int key2) const

  check for consistency in response map keys

- bool force_rebuild ()

  evaluate whether a rebuild of the approximation should be forced based on changes in the inactive data

- void asv_combine (const ShortArray &actual_asv, const ShortArray &approx_asv, ShortArray &combined_-asv)

  reconstitutes a combined_asv from actual_asv and approx_asv

- void response_combine (const Response &actual_response, const Response &approx_response, Response &combined_response)

  overlays actual_response and approx_response to update combined_response

- void aggregate_response (const Response &hf_resp, const Response &lf_resp, Response &agg_resp)

  aggregate {HF,LF} response data to create a new response with 2x size

- void insert_response (const Response &response, size_t position, Response &agg_response)

  insert a single response into an aggregated response in the specified position

Protected Attributes

- SizetSet surrogateFnIndices

  for mixed response sets, this array specifies the response function subset that is approximated
- short responseMode

  an enumeration that controls the response calculation mode in {DataFit,Hierarch}SurrModel approximate response computations
- Pecos::ActiveKey activeKey

  array of indices that identify the currently active model key
- short corrType

  type of correction: additive, multiplicative, or combined
- int surrModelEvalCntr

  counter for calls to derived_evaluate()/derived_evaluate_nowait(); used to key response maps from SurrogateModels
- IntResponseMap surrResponseMap

  map of surrogate responses returned by derived_synchronize() and derived_synchronize_nowait()
- size_t approxBuilds

  number of calls to build_approximation()
- size_t miPLIndex

  the index of the active metaiterator-iterator parallelism level (corresponding to ParallelConfiguration::miPLIters) used at runtime
- RealVector referenceCLBnds

  stores a reference copy of active continuous lower bounds when the approximation is built; used to detect when a rebuild is required.
- RealVector referenceCUBnds

  stores a reference copy of active continuous upper bounds when the approximation is built; used to detect when a rebuild is required.
- IntVector referenceDILBnds

  stores a reference copy of active discrete int lower bounds when the approximation is built; used to detect when a rebuild is required.
- IntVector referenceDIUBnds

  stores a reference copy of active discrete int upper bounds when the approximation is built; used to detect when a rebuild is required.
- RealVector referenceDRLBnds

  stores a reference copy of active discrete real lower bounds when the approximation is built; used to detect when a rebuild is required.
- RealVector referenceDRUBnds

  stores a reference copy of active discrete real upper bounds when the approximation is built; used to detect when a rebuild is required.
- RealVector referenceICVars

  stores a reference copy of the inactive continuous variables when the approximation is built using a Distinct view; used to detect when a rebuild is required.
- IntVector referenceIDIVars

  stores a reference copy of the inactive discrete int variables when the approximation is built using a Distinct view; used to detect when a rebuild is required.
- StringMultiArray referenceIDSVars

  stores a reference copy of the inactive discrete string variables when the approximation is built using a Distinct view; used to detect when a rebuild is required.
- RealVector referenceIDRVars

  stores a reference copy of the inactive discrete real variables when the approximation is built using a Distinct view; used to detect when a rebuild is required.

Private Member Functions

- void update_all_variables_from_model (const Model &model)

    update all current variables/bounds/labels with data from model
- void update_complement_variables_from_model (const Model &model)

    update complement of active variables/bounds with data from model

Private Attributes

- Variables truthModelVars

    copy of the truth model variables object used to simplify conversion among differing variable views in force_rebuild()
- Constraints truthModelCons

    copy of the truth model constraints object used to simplify conversion among differing variable views in force_rebuild()

Additional Inherited Members

14.275.1 Detailed Description

Base class for surrogate models (DataFitSurrModel and HierarchSurrModel).

The SurrogateModel class provides common functions to derived classes for computing and applying corrections to approximations.

14.275.2 Member Function Documentation

14.275.2.1 int derived_evaluation_id ( ) const [inline], [protected], [virtual]

return the current evaluation id for this Model

return the SurrogateModel evaluation id counter. Due to possibly intermittent use of lower level components, this is not the same as approxInterface, actualModel, or orderedModels evaluation counts, which requires a consistent evaluation rekeying process.

Reimplemented from Model.

References SurrogateModel::surrModelEvalCntr.

14.275.2.2 void update_from_model (const Model & *model*) [protected], [virtual]

update current variables/labels/bounds/targets with data from model

Update values and labels in currentVariables and bound/linear/nonlinear constraints in userDefinedConstraints from variables and constraints data within model.

Reimplemented in DataFitSurrModel.

References Model::is_null(), SurrogateModel::update_response_from_model(), and SurrogateModel::update_-variables_from_model().

Referenced by NonHierarchSurrModel::update_from_subordinate_model(), and HierarchSurrModel::update_from-_subordinate_model().

14.275.2.3 void init_model_constraints (Model & *model*) [protected]

initialize model with linear/nonlinear constraint data that could change once per set of evaluations (e.g., an outer iterator execution)

Update variables and constraints data within model using values and labels from currentVariables and bound/linear/nonlinear constraints from userDefinedConstraints.

References Dakota::abort_handler(), Model::currentVariables, Variables::cv(), Model::cv(), Variables::div(), Model::div(), Variables::drv(), Model::drv(), Variables::dsv(), Model::dsv(), Model::is_null(), Constraints::linear_eq_constraint_coeffs(), Model::linear_eq_constraint_coeffs(), Constraints::linear_eq_constraint_targets(), Model::linear_eq_constraint_targets(), Constraints::linear_ineq_constraint_coeffs(), Model::linear_ineq_constraint_coeffs(), Constraints::linear_ineq_constraint_lower_bounds(), Model::linear_ineq_constraint_lower_bounds(), Constraints::linear_ineq_constraint_upper_bounds(), Model::linear_ineq_constraint_upper_bounds(), Constraints::nonlinear_eq_constraint_targets(), Model::nonlinear_eq_constraint_targets(), Constraints::nonlinear_ineq_constraint_lower_bounds(), Model::nonlinear_ineq_constraint_lower_bounds(), Constraints::nonlinear_ineq_constraint_upper_bounds(), Model::nonlinear_ineq_constraint_upper_bounds(), Constraints::num_linear_eq_constraints(), Constraints::num_linear_ineq_constraints(), Constraints::num_nonlinear_eq_constraints(), Constraints::num_nonlinear_ineq_constraints(), and Model::userDefinedConstraints.

Referenced by SurrogateModel::init_model().

14.275.2.4 bool force_rebuild ( ) [protected], [virtual]

evaluate whether a rebuild of the approximation should be forced based on changes in the inactive data

This function forces a rebuild of the approximation according to the sub-model variables view, the approximation type, and whether the active approximation bounds or inactive variable values have changed since the last approximation build.

Reimplemented from Model.

References Constraints::all_continuous_lower_bounds(), Constraints::all_continuous_upper_bounds(), Variables::all_continuous_variables(), Constraints::all_discrete_int_lower_bounds(), Constraints::all_discrete_int_upper_bounds(), Variables::all_discrete_int_variables(), Constraints::all_discrete_real_lower_bounds(), Constraints::all_discrete_real_upper_bounds(), Variables::all_discrete_real_variables(), Variables::all_discrete_string_variables(), Constraints::continuous_lower_bounds(), Model::continuous_lower_bounds(), Constraints::continuous_upper_bounds(), Model::continuous_upper_bounds(), Variables::continuous_variables(), Constraints::copy(), Variables::copy(), Model::current_variables(), Model::currentVariables, Constraints::discrete_int_lower_bounds(), Model::discrete_int_lower_bounds(), Constraints::discrete_int_upper_bounds(), Model::discrete_int_upper_bounds(), Variables::discrete_int_variables(), Constraints::discrete_real_lower_bounds(), Model::discrete_real_lower_bounds(), Constraints::discrete_real_upper_bounds(), Model::discrete_real_upper_bounds(), Variables::discrete_real_variables(), Variables::discrete_string_variables(), Variables::inactive_continuous_variables(), Variables::inactive_discrete_int_variables(), Variables::inactive_discrete_real_variables(), Variables::inactive_discrete_string_variables(), Constraints::is_null(), Variables::is_null(), Model::is_null(), Model::model_type(), SurrogateModel::referenceCLBnds, SurrogateModel::referenceCUBnds, SurrogateModel::referenceDILBnds, SurrogateModel::referenceDIUBnds, SurrogateModel::referenceDRLBnds, SurrogateModel::referenceDRUBnds, SurrogateModel::referenceICVars, SurrogateModel::referenceIDIVars, SurrogateModel::referenceIDRVars, SurrogateModel::referenceIDSVars, Dakota::strbegins(), Model::subordinate_model(), Model::surrogateType, Model::truth_model(), SurrogateModel::truthModelCons, SurrogateModel::truthModelVars, Model::user_defined_constraints(), Model::userDefinedConstraints, and Variables::view().

Referenced by HierarchSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate(), HierarchSurrModel::derived_evaluate_nowait(), and DataFitSurrModel::derived_evaluate_nowait().

14.275.2.5 void update_complement_variables_from_model (const Model & *model*) [private]

update complement of active variables/bounds with data from model

Update values and labels in currentVariables and bound/linear/nonlinear constraints in userDefinedConstraints from variables and constraints data within model.

References Variables::acv(), Model::acv(), Variables::adiv(), Model::adiv(), Variables::adrv(), Model::adrv(), Variables::adsv(), Model::adsv(), Constraints::all_continuous_lower_bound(), Constraints::all_continuous_lower_bounds(), Constraints::all_continuous_upper_bound(), Constraints::all_continuous_upper_bounds(), Variables::all_continuous_variable(), Variables::all_continuous_variable_labels(), Variables::all_continuous_variables(), Constraints::all_discrete_int_lower_bound(), Constraints::all_discrete_int_lower_bounds(), Constraints::all_-discrete_int_upper_bound(), Constraints::all_discrete_int_upper_bounds(), Variables::all_discrete_int_variable(), Variables::all_discrete_int_variable_labels(), Variables::all_discrete_int_variables(), Constraints::all_discrete_real-_lower_bound(), Constraints::all_discrete_real_lower_bounds(), Constraints::all_discrete_real_upper_bound(), Constraints::all_discrete_real_upper_bounds(), Variables::all_discrete_real_variable(), Variables::all_discrete_real-_variable_labels(), Variables::all_discrete_real_variables(), Variables::all_discrete_string_variable(), Variables-::all_discrete_string_variable_labels(), Variables::all_discrete_string_variables(), Model::current_variables(), Model::currentVariables, Variables::cv(), Variables::cv_start(), Variables::div(), Variables::div_start(), Variables-::drv(), Variables::drv_start(), Variables::dsv(), Variables::dsv_start(), Dakota::find_index(), Model::user_defined_-constraints(), and Model::userDefinedConstraints.

Referenced by SurrogateModel::update_variables_from_model().

14.275.3 Member Data Documentation

14.275.3.1 short responseMode [protected]

an enumeration that controls the response calculation mode in {DataFit,Hierarch}SurrModel approximate response computations

SurrBasedLocalMinimizer toggles this mode since compute_correction() does not back out old corrections.

Referenced by NonHierarchSurrModel::active_model_key(), HierarchSurrModel::active_model_key(), Surrogate-Model::asv_split(), NonHierarchSurrModel::component_parallel_mode(), HierarchSurrModel::component_parallel-_mode(), NonHierarchSurrModel::create_tabular_datastream(), HierarchSurrModel::create_tabular_datastream(), DataFitSurrModel::DataFitSurrModel(), DataFitSurrModel::declare_sources(), NonHierarchSurrModel::derived-_auto_graphics(), HierarchSurrModel::derived_auto_graphics(), NonHierarchSurrModel::derived_evaluate(), HierarchSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate(), NonHierarchSurrModel::derived-_evaluate_nowait(), HierarchSurrModel::derived_evaluate_nowait(), DataFitSurrModel::derived_evaluate_nowait(), NonHierarchSurrModel::derived_set_communicators(), HierarchSurrModel::derived_set_communicators(), DataFit-SurrModel::derived_synchronize(), DataFitSurrModel::derived_synchronize_approx(), DataFitSurrModel::derived-_synchronize_nowait(), HierarchSurrModel::extract_model_keys(), HierarchSurrModel::HierarchSurrModel(), SurrogateModel::init_model_labels(), HierarchSurrModel::insert_metadata(), HierarchSurrModel::insert_response-_start(), EnsembleSurrModel::qoi(), DataFitSurrModel::qoi(), NonHierarchSurrModel::resize_from_subordinate-_model(), HierarchSurrModel::resize_from_subordinate_model(), NonHierarchSurrModel::resize_maps(), Non-HierarchSurrModel::resize_response(), HierarchSurrModel::resize_response(), NonHierarchSurrModel::serve-_run(), HierarchSurrModel::serve_run(), SurrogateModel::surrogate_response_mode(), EnsembleSurrModel-::surrogate_response_mode(), DataFitSurrModel::surrogate_response_mode(), SurrogateModel::Surrogate-Model(), HierarchSurrModel::update_from_subordinate_model(), and SurrogateModel::update_response_from-_model().

14.275.3.2 size_t approxBuilds [protected]

number of calls to build_approximation()

used as a flag to automatically build the approximation if one of the derived evaluate functions is called prior to build_approximation().

Referenced by DataFitSurrModel::approximation_coefficients(), HierarchSurrModel::build_approximation(), Data-FitSurrModel::build_global(), DataFitSurrModel::build_local_multipoint(), DataFitSurrModel::DataFitSurrModel(), HierarchSurrModel::derived_evaluate(), DataFitSurrModel::derived_evaluate(), HierarchSurrModel::derived_-evaluate_nowait(), DataFitSurrModel::derived_evaluate_nowait(), SurrogateModel::init_model_inactive_labels(), SurrogateModel::init_model_labels(), DataFitSurrModel::pop_approximation(), DataFitSurrModel::rebuild_-approximation(), DataFitSurrModel::rebuild_global(), SurrogateModel::update_all_variables_from_model(), and SurrogateModel::update_response_from_model().

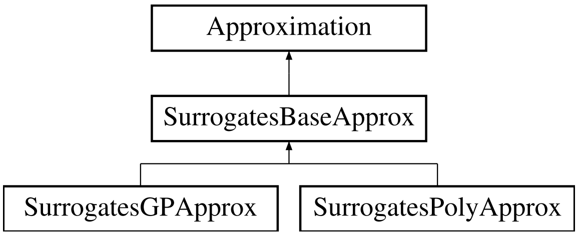
The documentation for this class was generated from the following files:

- SurrogateModel.hpp
- SurrogateModel.cpp

14.276 SurrogatesBaseApprox Class Reference

Derived Approximation class for new Surrogates modules.

Inheritance diagram for SurrogatesBaseApprox:



Public Member Functions

- SurrogatesBaseApprox ()
  default constructor
- SurrogatesBaseApprox (const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)
  standard constructor:
- SurrogatesBaseApprox (const SharedApproxData &shared_data)
  alternate constructor
- ∼SurrogatesBaseApprox ()
  destructor
- bool diagnostics_available () override
  check if diagnostics are available for this approximation type
- Real diagnostic (const String &metric_type) override
  retrieve a single diagnostic metric for the diagnostic type specified
- RealArray cv_diagnostic (const StringArray &metric_types, unsigned num_folds) override
  retrieve diagnostic metrics for the diagnostic types specified, applying
- void primary_diagnostics (size_t fn_index) override
  compute and print all requested diagnostics and cross-validation
- void challenge_diagnostics (size_t fn_index, const RealMatrix &challenge_points, const RealVector &challenge_responses) override
  compute and print all requested diagnostics for user provided challenge pts
- dakota::ParameterList & **getSurrogateOpts** ()

Protected Member Functions

- void convert_surrogate_data (dakota::MatrixXd &vars, dakota::MatrixXd &resp)
  convert Pecos surrogate data to reshaped Eigen vars/resp matrices
- Real value (const Variables &vars) override
  retrieve the approximate function value for a given parameter vector
- const RealVector & gradient (const Variables &vars) override
  retrieve the approximate function gradient for a given parameter vector
- Real value (const RealVector &c_vars) override
  retrieve the approximate function value for a given parameter vector
- const RealVector & gradient (const RealVector &c_vars) override
  retrieve the approximate function gradient for a given parameter vector
- void set_verbosity ()

set the surrogate's verbosity level according to Dakota's verbosity
- void import_model (const ProblemDescDB &problem_db)

  construct-time only import of serialized surrogate
- void map_variable_labels (const Variables &vars)

  validate imported labels and initialize map if needed
- RealVector map_eval_vars (const Variables &vars)

  extract active or all view as vector, mapping if needed for import
- void export_model (const StringArray &var_labels, const String &fn_label, const String &export_prefix, const unsigned short export_format) override

  export the model to disk
- void export_model (const Variables &vars, const String &fn_label, const String &export_prefix, const unsigned short export_format) override

  approximation export that generates labels from the passed Variables, since only the derived classes know how the variables are ordered w.r.t. the surrogate build; if export_format > NO_MODEL_FORMAT, uses all 3 parameters, otherwise extracts these from the Approximation's sharedDataRep to build a filename

Protected Attributes

- dakota::ParameterList surrogateOpts

  Key/value config options for underlying surrogate.
- std::shared_ptr
  < dakota::surrogates::Surrogate > model

  The native surrogate model.
- String advanced_options_file

  Advanced configurations options filename.
- bool modelIsImported

  whether model serialized in from disk

14.276.1 Detailed Description

Derived Approximation class for new Surrogates modules.

Encapsulates common behavior for Surrogates modules, with specialization for specific surrogates in derived classes.

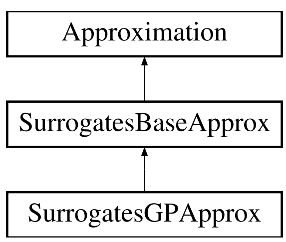
The documentation for this class was generated from the following files:

- DakotaSurrogates.hpp
- DakotaSurrogates.cpp

14.277 SurrogatesGPApprox Class Reference

Derived approximation class for Surrogates approximation classes.

Inheritance diagram for SurrogatesGPApprox:



Public Member Functions

- SurrogatesGPApprox ()
  default constructor
- SurrogatesGPApprox (const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)
  standard constructor:
- SurrogatesGPApprox (const SharedApproxData &shared_data)
  alternate constructor
- ∼SurrogatesGPApprox ()
  destructor

Protected Member Functions

- int min_coefficients () const override
  return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- void build () override
  Do the build.
- Real prediction_variance (const Variables &vars) override
  retrieve the variance of the predicted value for a given parameter vector
- Real prediction_variance (const RealVector &c_vars) override
  retrieve the variance of the predicted value for a given parameter vector

Additional Inherited Members

14.277.1 Detailed Description

Derived approximation class for Surrogates approximation classes.

This class interfaces Dakota to the Dakota Surrogates Gaussian Process Module.

14.277.2 Constructor & Destructor Documentation

14.277.2.1 SurrogatesGPApprox (const SharedApproxData & *shared_data*)

alternate constructor

On-the-fly constructor.

References SurrogatesBaseApprox::surrogateOpts.

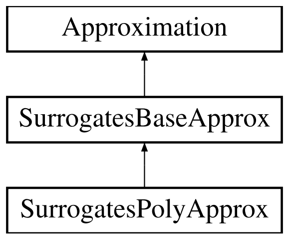
The documentation for this class was generated from the following files:

- DakotaSurrogatesGP.hpp
- DakotaSurrogatesGP.cpp

14.278 SurrogatesPolyApprox Class Reference

Derived approximation class for Surrogates Polynomial approximation classes.

Inheritance diagram for SurrogatesPolyApprox:



Public Member Functions

- SurrogatesPolyApprox ()

    default constructor
- SurrogatesPolyApprox (const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

    standard constructor:
- SurrogatesPolyApprox (const SharedApproxData &shared_data)

    alternate constructor
- ∼SurrogatesPolyApprox ()

    destructor

Protected Member Functions

- int min_coefficients () const override

    return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- void build () override

    Do the build.

Additional Inherited Members

14.278.1 Detailed Description

Derived approximation class for Surrogates Polynomial approximation classes.

This class interfaces Dakota to the Dakota Surrogates Polynomial Module.

14.278.2 Constructor & Destructor Documentation

14.278.2.1 SurrogatesPolyApprox (const SharedApproxData & *shared_data*)

alternate constructor

On-the-fly constructor.

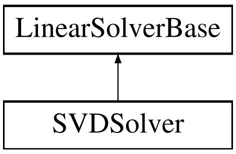
The documentation for this class was generated from the following files:

- DakotaSurrogatesPoly.hpp
- DakotaSurrogatesPoly.cpp

14.279 SVDSolver Class Reference

The SVDSolver class is used to solve linear systems with the singular value decomposition.

Inheritance diagram for SVDSolver:



Public Member Functions

- SVDSolver ()

    Constructor.
- ∼SVDSolver ()

    Destructor.
- bool is_factorized () const override

    Query to determine if the matrix of the solver has been factored.
- void factorize (const MatrixXd &A) override

    Perform the matrix factorization for the linear solver matrix.
- void solve (const MatrixXd &A, const MatrixXd &b, MatrixXd &x) override

    Find a solution to Ax = b.
- void solve (const MatrixXd &b, MatrixXd &x) override

    Find a solution to Ax = b when A is already factorized.

Private Attributes

- std::shared_ptr< Eigen::BDCSVD
  < MatrixXd > > **SVD_Ptr**

Additional Inherited Members

14.279.1 Detailed Description

The SVDSolver class is used to solve linear systems with the singular value decomposition.

14.279.2 Member Function Documentation

14.279.2.1 void factorize (const MatrixXd & *A*) [override], [virtual]

Perform the matrix factorization for the linear solver matrix.

Parameters

in	*A*	The incoming matrix to factorize.

Reimplemented from LinearSolverBase.

Referenced by SVDSolver::solve().

14.279.2.2 void solve (const MatrixXd & *A*, const MatrixXd & *b*, MatrixXd & *x*) [override], [virtual]

Find a solution to Ax = b.

Parameters

in	*A*	The linear system left-hand-side matrix.
in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented from LinearSolverBase.

References SVDSolver::factorize().

14.279.2.3 void solve (const MatrixXd & *b*, MatrixXd & *x*) [override], [virtual]

Find a solution to Ax = b when A is already factorized.

Parameters

in	*b*	The linear system right-hand-side (multi-)vector.
in	*x*	The linear system solution (multi-)vector.

Reimplemented from LinearSolverBase.

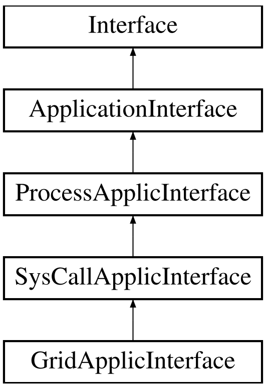
The documentation for this class was generated from the following files:

- UtilLinearSolvers.hpp
- UtilLinearSolvers.cpp

14.280 SysCallApplicInterface Class Reference

Derived application interface class which spawns simulation codes using system calls.

Inheritance diagram for SysCallApplicInterface:



Public Member Functions

- SysCallApplicInterface (const ProblemDescDB &problem_db)

  constructor
- ∼SysCallApplicInterface ()

  destructor

Protected Member Functions

- void wait_local_evaluation_sequence (PRPQueue &prp_queue)
- void test_local_evaluation_sequence (PRPQueue &prp_queue)

- int synchronous_local_analysis (int analysis_id)
- void init_communicators_checks (int max_eval_concurrency)
- void set_communicators_checks (int max_eval_concurrency)
- void map_bookkeeping (pid_t pid, int fn_eval_id)

  bookkeeping of process and evaluation ids for asynchronous maps
- pid_t create_evaluation_process (bool block_flag)

  Spawn the evaluation by managing the input filter, analysis drivers, and output filter. Called from derived_map() & derived_map_asynch().

Private Member Functions

- bool system_call_file_test (const bfs::path &root_file)

  detect completion of a function evaluation through existence of the necessary results file(s); return true if results files found
- void spawn_evaluation_to_shell (bool block_flag)

  spawn a complete function evaluation
- void spawn_input_filter_to_shell (bool block_flag)

  spawn the input filter portion of a function evaluation
- void spawn_analysis_to_shell (int analysis_id, bool block_flag)

  spawn a single analysis as part of a function evaluation
- void spawn_output_filter_to_shell (bool block_flag)

  spawn the output filter portion of a function evaluation

Private Attributes

- IntSet sysCallSet

  set of function evaluation id's for active asynchronous system call evaluations
- IntShortMap failCountMap

  map linking function evaluation id's to number of response read failures

Additional Inherited Members

14.280.1 Detailed Description

Derived application interface class which spawns simulation codes using system calls.

system() is part of the C API and can be used on both Windows and Unix systems.

14.280.2 Member Function Documentation

14.280.2.1 void wait_local_evaluation_sequence (PRPQueue & *prp_queue*) [inline], [protected], [virtual]

Check for completion of active asynch jobs (tracked with sysCallSet). Wait for at least one completion and complete all jobs that have returned. This satisifies a "fairness" principle, in the sense that a completed job will *always* be processed (whereas accepting only a single completion could always accept the same completion - the case of very inexpensive fn. evals. - and starve some servers).

Implements ProcessApplicInterface.

References ApplicationInterface::completionSet, and SysCallApplicInterface::test_local_evaluation_sequence().

14.280.2.2 void test_local_evaluation_sequence (PRPQueue & *prp_queue*) [protected], [virtual]

Check for completion of active asynch jobs (tracked with sysCallSet). Make one pass through sysCallSet & complete all jobs that have returned.

Implements ProcessApplicInterface.

References Dakota::abort_handler(), Response::active_set(), ApplicationInterface::completionSet, SysCallApplicInterface::failCountMap, ProcessApplicInterface::fileNameMap, ApplicationInterface::final_eval_id_tag(), Dakota::lookup_by_eval_id(), ApplicationInterface::manage_failure(), ProcessApplicInterface::read_results_files(), SysCallApplicInterface::sysCallSet, and SysCallApplicInterface::system_call_file_test().

Referenced by SysCallApplicInterface::wait_local_evaluation_sequence().

14.280.2.3 int synchronous_local_analysis (int *analysis_id*) [inline], [protected], [virtual]

This code provides the derived function used by ApplicationInterface::serve_analyses_synch().

Reimplemented from ApplicationInterface.

References SysCallApplicInterface::spawn_analysis_to_shell().

14.280.2.4 void init_communicators_checks (int *max_eval_concurrency*) [inline], [protected], [virtual]

No derived interface plug-ins, so perform construct-time checks. However, process init issues as warnings since some contexts (e.g., HierarchSurrModel) initialize more configurations than will be used.

Reimplemented from ApplicationInterface.

References ApplicationInterface::check_multiprocessor_analysis().

14.280.2.5 void set_communicators_checks (int *max_eval_concurrency*) [inline], [protected], [virtual]

Process run-time issues as hard errors.

Reimplemented from ApplicationInterface.

References Dakota::abort_handler(), and ApplicationInterface::check_multiprocessor_analysis().

14.280.2.6 void spawn_evaluation_to_shell (bool *block_flag*) [private]

spawn a complete function evaluation

Put the SysCallApplicInterface to the shell. This function is used when all portions of the function evaluation (i.e., all analysis drivers) are executed on the local processor.

References CommandShell::asynch_flag(), ProcessApplicInterface::commandLineArgs, ProcessApplicInterface::curWorkdir, Dakota::flush(), ProcessApplicInterface::iFilterName, ProcessApplicInterface::multipleParamsFiles, ProcessApplicInterface::oFilterName, ProcessApplicInterface::paramsFileName, ProcessApplicInterface::prepare_process_environment(), ProcessApplicInterface::programNames, ProcessApplicInterface::reset_process_environment(), ProcessApplicInterface::resultsFileName, Dakota::substitute_params_and_results(), CommandShell::suppress_output_flag(), ApplicationInterface::suppressOutput, and ProcessApplicInterface::useWorkdir.

Referenced by SysCallApplicInterface::create_evaluation_process().

14.280.2.7 void spawn_input_filter_to_shell (bool *block_flag*) [private]

spawn the input filter portion of a function evaluation

Put the input filter to the shell. This function is used when multiple analysis drivers are spread between processors. No need to check for a Null input filter, as this is checked externally. Use of nonblocking shells is supported in this fn, although its use is currently prevented externally.

References CommandShell::asynch_flag(), ProcessApplicInterface::commandLineArgs, Dakota::flush(), ProcessApplicInterface::iFilterName, ProcessApplicInterface::paramsFileName, ProcessApplicInterface::prepare_process_environment(), ProcessApplicInterface::reset_process_environment(), ProcessApplicInterface::resultsFileName, Dakota::substitute_params_and_results(), CommandShell::suppress_output_flag(), and ApplicationInterface::suppressOutput.

Referenced by SysCallApplicInterface::create_evaluation_process().

14.280.2.8 void spawn_analysis_to_shell (int *analysis_id,* bool *block_flag*) [private]

spawn a single analysis as part of a function evaluation

Put a single analysis to the shell. This function is used when multiple analysis drivers are spread between processors. Use of nonblocking shells is supported in this fn, although its use is currently prevented externally.

References CommandShell::asynch_flag(), ProcessApplicInterface::commandLineArgs, Dakota::flush(), ProcessApplicInterface::multipleParamsFiles, ProcessApplicInterface::paramsFileName, ProcessApplicInterface::prepare_process_environment(), ProcessApplicInterface::programNames, ProcessApplicInterface::reset_process_environment(), ProcessApplicInterface::resultsFileName, Dakota::substitute_params_and_results(), CommandShell::suppress_output_flag(), and ApplicationInterface::suppressOutput.

Referenced by SysCallApplicInterface::create_evaluation_process(), SysCallApplicInterface::synchronous_local_analysis(), and GridApplicInterface::synchronous_local_analysis().

14.280.2.9 void spawn_output_filter_to_shell (bool *block_flag*) [private]

spawn the output filter portion of a function evaluation

Put the output filter to the shell. This function is used when multiple analysis drivers are spread between processors. No need to check for a Null output filter, as this is checked externally. Use of nonblocking shells is supported in this fn, although its use is currently prevented externally.

References CommandShell::asynch_flag(), ProcessApplicInterface::commandLineArgs, Dakota::flush(), ProcessApplicInterface::oFilterName, ProcessApplicInterface::paramsFileName, ProcessApplicInterface::prepare_process_environment(), ProcessApplicInterface::reset_process_environment(), ProcessApplicInterface::resultsFileName, Dakota::substitute_params_and_results(), CommandShell::suppress_output_flag(), and ApplicationInterface::suppressOutput.

Referenced by SysCallApplicInterface::create_evaluation_process().

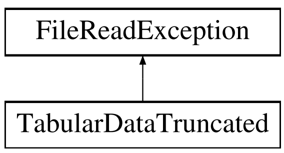
The documentation for this class was generated from the following files:

- SysCallApplicInterface.hpp
- SysCallApplicInterface.cpp

14.281 TabularDataTruncated Class Reference

exception thrown when data read truncated

Inheritance diagram for TabularDataTruncated:



Public Member Functions

- **TabularDataTruncated** (const std::string &msg)

14.281.1 Detailed Description

exception thrown when data read truncated

The documentation for this class was generated from the following file:

- dakota_global_defs.hpp

14.282 TabularReader Class Reference

Utility used in derived read_core to read values in tabular format.

Public Member Functions

- template<typename ArrayType >
  void operator() (std::istream &s, size_t start_index, size_t num_items, ArrayType &array_data, StringMultiArrayView label_array)

14.282.1 Detailed Description

Utility used in derived read_core to read values in tabular format.

14.282.2 Member Function Documentation

14.282.2.1 void operator() (std::istream & *s*, size_t *start_index*, size_t *num_items*, ArrayType & *array_data*, StringMultiArrayView *label_array*) [inline]

The tabular reader doesn't forward the label arrays

The documentation for this class was generated from the following file:

- DakotaVariables.hpp

14.283 TabularWriter Class Reference

Utility used in derived write_core to write values in tabular format.

Public Member Functions

- template<typename ArrayType >
  void operator() (std::ostream &s, size_t start_index, size_t num_items, const ArrayType &array_data, StringMultiArrayConstView label_array)

14.283.1 Detailed Description

Utility used in derived write_core to write values in tabular format.

14.283.2 Member Function Documentation

14.283.2.1 void operator() (std::ostream & *s*, size_t *start_index*, size_t *num_items*, const ArrayType & *array_data*, StringMultiArrayConstView *label_array*) [inline]

The tabular writer doesn't forward the label arrays

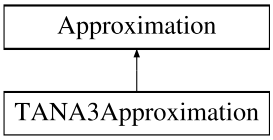
The documentation for this class was generated from the following file:

- DakotaVariables.hpp

14.284 TANA3Approximation Class Reference

Derived approximation class for TANA-3 two-point exponential approximation (a multipoint approximation).

Inheritance diagram for TANA3Approximation:



Public Member Functions

- TANA3Approximation ()

  default constructor
- TANA3Approximation (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

  standard constructor
- TANA3Approximation (const SharedApproxData &shared_data)

  alternate constructor
- ∼TANA3Approximation ()

  destructor

Protected Member Functions

- int min_coefficients () const

  return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- void build ()

  builds the approximation from scratch
- Real value (const Variables &vars)

  retrieve the approximate function value for a given parameter vector
- const RealVector & gradient (const Variables &vars)

  retrieve the approximate function gradient for a given parameter vector
- void clear_current_active_data ()

Private Member Functions

- void find_scaled_coefficients ()

    compute TANA coefficients based on scaled inputs
- void offset (const RealVector &x, RealVector &s)

    based on minX, offset original parameters (x) to define positive parameters (s)

Private Attributes

- RealVector pExp

    vector of exponent values
- RealVector minX

    vector of minimum param values used for offset/scaling
- RealVector scX1

    vector of scaled and/or offset x1 values
- RealVector scX2

    vector of scaled and/or offset x2 values
- Real H

    the scalar Hessian value in the TANA-3 approximation

Additional Inherited Members

14.284.1 Detailed Description

Derived approximation class for TANA-3 two-point exponential approximation (a multipoint approximation).

The TANA3Approximation class provides a multipoint approximation based on matching value and gradient data from two points (typically the current and previous iterates) in parameter space. It forms an exponential approximation in terms of intervening variables.

14.284.2 Member Function Documentation

14.284.2.1 void build ( ) [protected], [virtual]

builds the approximation from scratch

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

References Dakota::abort_handler(), Approximation::approxData, Approximation::build(), TANA3Approximation::find_scaled_coefficients(), Dakota::length(), TANA3Approximation::minX, TANA3Approximation::pExp, and Approximation::sharedDataRep.

14.284.2.2 void clear_current_active_data ( ) [inline], [protected], [virtual]

Redefine default implementation to support history mechanism.

Reimplemented from Approximation.

References Approximation::approxData, and Approximation::sharedDataRep.

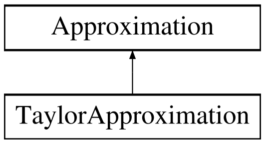
The documentation for this class was generated from the following files:

- TANA3Approximation.hpp
- TANA3Approximation.cpp

14.285 TaylorApproximation Class Reference

Derived approximation class for first- or second-order Taylor series (a local approximation).

Inheritance diagram for TaylorApproximation:



Public Member Functions

- TaylorApproximation ()

  default constructor
- TaylorApproximation (ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

  standard constructor
- TaylorApproximation (const SharedApproxData &shared_data)

  alternate constructor
- ∼TaylorApproximation ()

  destructor

Protected Member Functions

- int min_coefficients () const

  return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- void build ()

  builds the approximation from scratch
- Real value (const Variables &vars)

  retrieve the approximate function value for a given parameter vector
- const RealVector & gradient (const Variables &vars)

  retrieve the approximate function gradient for a given parameter vector
- const RealSymMatrix & hessian (const Variables &vars)

  retrieve the approximate function Hessian for a given parameter vector

Additional Inherited Members

14.285.1 Detailed Description

Derived approximation class for first- or second-order Taylor series (a local approximation).

The TaylorApproximation class provides a local approximation based on data from a single point in parameter space. It uses a zeroth-, first- or second-order Taylor series expansion: f(x) = f(x_c) for zeroth-order, plus grad(x_c)' (x - x_c) for first- and second-order, and plus (x - x_c)' Hess(x_c) (x - x_c) / 2 for second-order.

14.285.2 Member Function Documentation

14.285.2.1 void build ( ) [protected], [virtual]

builds the approximation from scratch

This is the common base class portion of the virtual fn and is insufficient on its own; derived implementations should explicitly invoke (or reimplement) this base class contribution.

Reimplemented from Approximation.

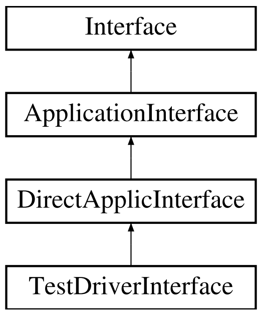
References Dakota::abort_handler(), Approximation::approxData, Approximation::build(), and Approximation::sharedDataRep.

The documentation for this class was generated from the following files:

- TaylorApproximation.hpp
- TaylorApproximation.cpp

14.286 TestDriverInterface Class Reference

Inheritance diagram for TestDriverInterface:



Public Member Functions

- TestDriverInterface (const ProblemDescDB &problem_db)

    constructor
- ∼TestDriverInterface ()

    destructor

Protected Member Functions

- virtual int derived_map_ac (const Dakota::String &ac_name)

    execute an analysis code portion of a direct evaluation invocation

Private Member Functions

- int cantilever ()

    scaled cantilever test function for optimization
- int mod_cantilever ()

    unscaled cantilever test function for UQ
- int cantilever_ml ()

    unscaled cantilever test function for UQ with levels

- int cyl_head ()

  the cylinder head constrained optimization test fn
- int multimodal ()

  multimodal UQ test function
- int log_ratio ()

  the log_ratio UQ test function
- int short_column ()

  the short_column UQ/OUU test function
- int lf_short_column ()

  a low fidelity short_column test function
- int mf_short_column ()

  alternate short_column formulations for < multifidelity or model form studies
- int alternate_short_column_forms (int form)

  helper fn for alternate forms
- int side_impact_cost ()

  the side_impact_cost UQ/OUU test function
- int side_impact_perf ()

  the side_impact_perf UQ/OUU test function
- int rosenbrock ()

  the Rosenbrock optimization and least squares test fn
- int modified_rosenbrock ()

  `the modified Rosenbrock optimization and`
  least squares test fn. The modification is the addition of an sin^2 term so that function can not be exactly approximated by a low degree polynomial
- int generalized_rosenbrock ()

  n-dimensional Rosenbrock (Schittkowski)
- int extended_rosenbrock ()

  n-dimensional Rosenbrock (Nocedal/Wright)
- int lf_rosenbrock ()

  a low fidelity version of the Rosenbrock function
- int extra_lf_rosenbrock ()

  an extra low fidelity version of the Rosenbrock function
- int mf_rosenbrock ()

  alternate Rosenbrock formulations for < multifidelity or model form studies
- int lf_poly_prod ()

  modified low fidelity Rosenbrock to test SBO with < hierarchical approximations
- int poly_prod ()

  modified low fidelity Rosenbrock to test SBO with < hierarchical approximations
- int gerstner ()

  the isotropic/anisotropic Gerstner test function family
- int scalable_gerstner ()

  scalable versions of the Gerstner test family
- void get_genz_coefficients (int num_dims, Real factor, int c_type, RealVector &c, RealVector &w)

  define coefficients needs for genz model
- int genz ()

  scalable test functions from the Genz test suite
- int damped_oscillator ()

  1d-6d that returns field values (ode solution)
- int steady_state_diffusion_1d ()

  solve the 1d steady-state diffusion eqn < with uncertain field diffusivity
- int ss_diffusion_discrepancy ()

difference steady_state_diffusion_1d() < across two consecutive resolutions
- int transient_diffusion_1d ()

  solve the 1d transient diffusion equation < with uncertain scalar diffusivity
- int **tunable_model** ()
- int predator_prey ()

  3 model hierarchy with tunable hyper-parameter(s)
- int steel_column_cost ()

  solve a predator prey population dynamics model
- int steel_column_perf ()

  the steel_column_perf UQ/OUU test function
- int sobol_rational ()

  Sobol SA rational test function.
- int sobol_g_function ()

  Sobol SA discontinuous test function.
- int sobol_ishigami ()

  Sobol SA transcendental test function.
- int text_book ()

  the text_book constrained optimization test function
- int text_book1 ()

  portion of text_book() evaluating the objective fn
- int text_book2 ()

  portion of text_book() evaluating constraint 1
- int text_book3 ()

  portion of text_book() evaluating constraint 2
- int text_book_ouu ()

  the text_book_ouu OUU test function
- int scalable_text_book ()

  scalable version of the text_book test function
- int scalable_monomials ()

  simple monomials for UQ exactness testing
- int mogatest1 ()

  MOP2 from Van Veldhuizen, pp. 5-13.
- int mogatest2 ()

  MOP2? from Van Veldhuizen, pp. 5-13.
- int mogatest3 ()

  Srinivas' from Van Veldhuizen, pp. B-5.
- int illumination ()

  illumination example in Boyd as a general < minimization problem
- int barnes ()

  barnes test for SBO perforamnce from Rodriguez, < Perez, Renaud, et al.
- int barnes_lf ()

  lo-fi barnes test for SBO perforamnce
- void herbie1D (size_t der_mode, Real xc_loc, std::vector< Real > &w_and_ders)

  1D components of herbie function
- void smooth_herbie1D (size_t der_mode, Real xc_loc, std::vector< Real > &w_and_ders)

  1D components of smooth_herbie function
- void shubert1D (size_t der_mode, Real xc_loc, std::vector< Real > &w_and_ders)

  1D components of shubert function
- int herbie ()

  returns the N-D herbie function
- int smooth_herbie ()

returns the N-D smooth herbie function

- int shubert ()

  returns the N-D shubert function

- int bayes_linear ()

  Scalable test function for Bayesian methods, to estimate parameters.

- int **problem18** ()
- double **problem18_f** (const double &x)
- double **problem18_g** (const double &x)
- double **problem18_Ax** (const double &A, const double &x)
- void separable_combine (Real mult_scale_factor, std::vector< Real > &w, std::vector< Real > &d1w, std::vector< Real > &d2w)

  utility to combine components of separable fns

- Real levenshtein_distance (const String &v)

  Compute Levenshtein distance between v and LEV_REF.

- int salinas ()

  direct interface to the SALINAS structural dynamics code

- int mc_api_run ()

  direct interface to ModelCenter via API, HKIM 4/3/03

- int aniso_quad_form ()

  1-D function using a anisotropic quadratic form

- void steady_state_diffusion_core (SpectralDiffusionModel &model, RealVector &domain_limits)

  shared helper function between steady_state_diffusion_1d() and ss_diffusion_discrepancy()

Static Private Attributes

- static StringRealMap levenshteinDistanceCache

  Cache results of Levenshtein distance calc for efficiency.

Additional Inherited Members

14.286.1 Detailed Description

Specialization of DirectApplicInterface to embed algebraic test function drivers directly in Dakota

14.286.2 Member Function Documentation

14.286.2.1 int derived_map_ac (const Dakota::String & *ac_name*) [protected], [virtual]

execute an analysis code portion of a direct evaluation invocation

Derived map to evaluate a particular built-in test analysis function

Reimplemented from DirectApplicInterface.

References Dakota::abort_handler(), ApplicationInterface::analysisServerId, TestDriverInterface::aniso_quad_form(), TestDriverInterface::barnes(), TestDriverInterface::barnes_lf(), TestDriverInterface::bayes_linear(), TestDriverInterface::cantilever(), TestDriverInterface::cantilever_ml(), TestDriverInterface::cyl_head(), TestDriverInterface::damped_oscillator(), DirectApplicInterface::driverTypeMap, TestDriverInterface::extended_rosenbrock(), TestDriverInterface::extra_lf_rosenbrock(), TestDriverInterface::generalized_rosenbrock(), TestDriverInterface::genz(), TestDriverInterface::gerstner(), TestDriverInterface::herbie(), TestDriverInterface::illumination(), TestDriverInterface::lf_poly_prod(), TestDriverInterface::lf_rosenbrock(), TestDriverInterface::lf_short_column(), TestDriverInterface::log_ratio(), TestDriverInterface::mc_api_run(), TestDriverInterface::mf_rosenbrock(), TestDriverInterface::mf_short_column(), TestDriverInterface::mod_cantilever(), TestDriverInterface::modified_rosenbrock(), TestDriverInterface::mogatest1(), TestDriverInterface::mogatest2(), TestDriverInterface::mogatest3(), TestDriver-Interface::multimodal(), TestDriverInterface::poly_prod(), TestDriverInterface::predator_prey(), TestDriverInterface-::rosenbrock(), TestDriverInterface::salinas(), TestDriverInterface::scalable_gerstner(), TestDriverInterface-::scalable_monomials(), TestDriverInterface::scalable_text_book(), TestDriverInterface::short_column(), Test-DriverInterface::shubert(), TestDriverInterface::side_impact_cost(), TestDriverInterface::side_impact_perf(), Test-DriverInterface::smooth_herbie(), TestDriverInterface::sobol_g_function(), TestDriverInterface::sobol_ishigami(), TestDriverInterface::sobol_rational(), TestDriverInterface::ss_diffusion_discrepancy(), TestDriverInterface::steady-_state_diffusion_1d(), TestDriverInterface::steel_column_cost(), TestDriverInterface::steel_column_perf(), Test-DriverInterface::text_book(), TestDriverInterface::text_book1(), TestDriverInterface::text_book2(), TestDriver-Interface::text_book3(), TestDriverInterface::text_book_ouu(), and TestDriverInterface::transient_diffusion_1d().

14.286.2.2 int lf_poly_prod ( ) [private]

modified low fidelity Rosenbrock to test SBO with < hierarchical approximations

modified lo-fi Rosenbrock to test SBO with hierarchical approximations

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::fnGrads, Direct-ApplicInterface::fnHessians, DirectApplicInterface::fnVals, DirectApplicInterface::gradFlag, DirectApplicInterface-::hessFlag, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface-::numADIV, DirectApplicInterface::numADRV, DirectApplicInterface::numFns, and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

14.286.2.3 int poly_prod ( ) [private]

modified low fidelity Rosenbrock to test SBO with < hierarchical approximations

modified lo-fi Rosenbrock to test SBO with hierarchical approximations

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::fnGrads, Direct-ApplicInterface::fnHessians, DirectApplicInterface::fnVals, DirectApplicInterface::gradFlag, DirectApplicInterface-::hessFlag, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface-::numADIV, DirectApplicInterface::numADRV, DirectApplicInterface::numFns, and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

14.286.2.4 int steady_state_diffusion_1d ( ) [private]

solve the 1d steady-state diffusion eqn < with uncertain field diffusivity

Solve the 1D diffusion equation with an uncertain variable coefficient using the spectral Chebyshev collocation method.

del(k del(u)) = f on [0,1] subject to u(0) = 0 u(1) = 0

Here we set f = -1 and k = 1+4.∗sum_d [cos(2∗pi∗x)/(pi∗d)^2∗z[d]] d=1,...,num_dims where z_d are random variables, typically i.i.d uniform[-1,1]

References Dakota::abort_handler(), Dakota::find_index(), DirectApplicInterface::fnVals, TestDriverInterface-::steady_state_diffusion_core(), DirectApplicInterface::xC, DirectApplicInterface::xDI, DirectApplicInterface::xDI-Labels, DirectApplicInterface::xDS, and DirectApplicInterface::xDSLabels.

Referenced by TestDriverInterface::derived_map_ac().

14.286.2.5 int steel_column_cost ( ) [private]

solve a predator prey population dynamics model

the steel_column_cost UQ/OUU test function

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, DirectApplicInterface::fnVals, DirectApplicInterface::numDerivVars, DirectApplicInterface::numFns, DirectApplicInterface::numVars, DirectApplicInterface::varTypeDVV, and DirectApplicInterface::xCM.

Referenced by TestDriverInterface::derived_map_ac().

14.286.2.6 int barnes ( ) [private]

barnes test for SBO perforamnce from Rodriguez, $<$ Perez, Renaud, et al.

barnes test for SBO perforamnce from Rodriguez, Perez, Renaud, et al. Modified 3/7/18 to incorporate random a[].

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnVals, DirectApplicInterface::gradFlag, DirectApplicInterface::hessFlag, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface::numADIV, DirectApplicInterface::numADRV, DirectApplicInterface::numDerivVars, DirectApplicInterface::numFns, and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

14.286.2.7 int barnes_lf ( ) [private]

lo-fi barnes test for SBO perforamnce

lo-fi barnes test for SBO perforamnce from Rodriguez, Perez, Renaud, et al.

References Dakota::abort_handler(), DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnVals, DirectApplicInterface::gradFlag, DirectApplicInterface::hessFlag, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface::numADIV, DirectApplicInterface::numADRV, DirectApplicInterface::numDerivVars, DirectApplicInterface::numFns, and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

14.286.2.8 void herbie1D (size_t *der_mode,* Real *xc_loc,* std::vector$<$ Real $>$ & *w_and_ders*) [private]

1D components of herbie function

1D Herbie function and its derivatives (apart from a multiplicative factor)

Referenced by TestDriverInterface::herbie().

14.286.2.9 void smooth_herbie1D (size_t *der_mode,* Real *xc_loc,* std::vector$<$ Real $>$ & *w_and_ders*) [private]

1D components of smooth_herbie function

1D Smoothed Herbie= 1DHerbie minus the high frequency sine term, and its derivatives (apart from a multiplicative factor)

Referenced by TestDriverInterface::smooth_herbie().

14.286.2.10 void shubert1D (size_t *der_mode,* Real *xc_loc,* std::vector$<$ Real $>$ & *w_and_ders*) [private]

1D components of shubert function

1D Shubert function and its derivatives (apart from a multiplicative factor)

Referenced by TestDriverInterface::shubert().

14.286.2.11 int herbie ( ) [private]

returns the N-D herbie function

N-D Herbie function and its derivatives.

References DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, TestDriverInterface::herbie1-D(), DirectApplicInterface::numDerivVars, DirectApplicInterface::numVars, TestDriverInterface::separable_-combine(), and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

14.286.2.12 int smooth_herbie ( ) [private]

returns the N-D smooth herbie function

N-D Smoothed Herbie function and its derivatives.

References DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::num-DerivVars, DirectApplicInterface::numVars, TestDriverInterface::separable_combine(), TestDriverInterface::smooth-_herbie1D(), and DirectApplicInterface::xC.

Referenced by TestDriverInterface::derived_map_ac().

14.286.2.13 void separable_combine (Real *mult_scale_factor,* std::vector< Real > & *w,* std::vector< Real > & *d1w,* std::vector< Real > & *d2w*) [private]

utility to combine components of separable fns

this function combines N 1D functions and their derivatives to compute a N-D separable function and its derivatives, logic is general enough to support different 1D functions in different dimensions (can mix and match)

References DirectApplicInterface::directFnASV, DirectApplicInterface::directFnDVV, DirectApplicInterface::fnGrads, DirectApplicInterface::fnHessians, DirectApplicInterface::fnVals, DirectApplicInterface::numDerivVars, and Direct-ApplicInterface::numVars.

Referenced by TestDriverInterface::herbie(), TestDriverInterface::shubert(), and TestDriverInterface::smooth_-herbie().

14.286.2.14 Real levenshtein_distance (const String & *v*) [private]

Compute Levenshtein distance between v and LEV_REF.

Levenshtein distance is the number of changes (single character

References Dakota::LEV_REF, and TestDriverInterface::levenshteinDistanceCache.

Referenced by TestDriverInterface::text_book1(), TestDriverInterface::text_book2(), and TestDriverInterface::text_-book3().

14.286.2.15 int mc_api_run ( ) [private]

direct interface to ModelCenter via API, HKIM 4/3/03

The ModelCenter interface doesn't have any specific construct vs. run time functions. For now, we manage it along with the integrated test drivers

References Dakota::abort_handler(), Interface::analysisComponents, DirectApplicInterface::analysisDriverIndex, Dakota::dc_ptr_int, DirectApplicInterface::directFnASV, Interface::fnLabels, DirectApplicInterface::fnVals, Dakota-::mc_ptr_int, ApplicationInterface::multiProcAnalysisFlag, DirectApplicInterface::numACV, DirectApplicInterface-::numADIV, DirectApplicInterface::numADRV, DirectApplicInterface::numFns, DirectApplicInterface::xC, Direct-ApplicInterface::xCLabels, DirectApplicInterface::xDI, DirectApplicInterface::xDILabels, DirectApplicInterface::xDR, and DirectApplicInterface::xDRLabels.

Referenced by TestDriverInterface::derived_map_ac().

The documentation for this class was generated from the following files:

- TestDriverInterface.hpp
- TestDriverInterface.cpp

14.287 TKFactoryDIPC Class Reference

Custom RW TKfactory: passes Dakota QUESO instance pointer to the TK at build.

Inherits TransitionKernelFactory.

Public Member Functions

- TKFactoryDIPC (const std::string &name)

  Constructor for Dakota RW transition kernel factory.
- virtual ∼TKFactoryDIPC ()

  Destructor for Dakota RW transition kernel factory.
- void set_callback (NonDQUESOBayesCalibration ∗queso_instance)

  Update the factory's QUESO callback pointer.

Protected Member Functions

- virtual QUESO::SharedPtr
  < QUESO::BaseTKGroup
  < QUESO::GslVector,
  QUESO::GslMatrix > >::Type build_tk () override

  build and return the custom TK

Private Attributes

- NonDQUESOBayesCalibration ∗ nonDQUESOInstance

  pointer for callbacks to Dakota QUESO class

14.287.1 Detailed Description

Custom RW TKfactory: passes Dakota QUESO instance pointer to the TK at build.

Can't share this factory between random walk and logit as their constructor arguments differ

The documentation for this class was generated from the following file:

- QUESOImpl.hpp

14.288 TKFactoryDIPCLogit Class Reference

Custom Logit RW TKfactory: passed Dakota QUESO instance pointer to the TK at build.

Inherits TransitionKernelFactory.

Public Member Functions

- TKFactoryDIPCLogit (const std::string &name)

  Constructor for Dakota Logit RW transition kernel factory.
- virtual ∼TKFactoryDIPCLogit ()

  Destructor for Dakota Logit RW transition kernel factory.
- void set_callback (NonDQUESOBayesCalibration ∗queso_instance)

  Update the factory's QUESO callback pointer.

Protected Member Functions

- virtual QUESO::SharedPtr
  < QUESO::BaseTKGroup
  < QUESO::GslVector,
  QUESO::GslMatrix > >::Type build_tk () override

  build and return the custom TK

Private Attributes

- NonDQUESOBayesCalibration ∗ nonDQUESOInstance

  pointer for callbacks to Dakota QUESO class

14.288.1 Detailed Description

Custom Logit RW TKfactory: passed Dakota QUESO instance pointer to the TK at build.

Can't share this factory between random walk and logit as their constructor arguments differ

The documentation for this class was generated from the following file:

- QUESOImpl.hpp

14.289 TPLDataTransfer Class Reference

Public Member Functions

- TPLDataTransfer ()

  default constructor
- ∼TPLDataTransfer ()

  destructor
- void configure_data_adapters (std::shared_ptr< TraitsBase >, const Model &)

  Construct maps, etc. needed to exchange data to/from Dakota and the TPL.
- int num_dakota_nonlin_eq_constraints () const

  Number of nonlinear equality constraints from Dakota perspective.
- int num_tpl_nonlin_eq_constraints () const

  Number of nonlinear equality constraints from TPL perspective.
- int num_dakota_nonlin_ineq_constraints () const

  Number of nonlinear inequality constraints from Dakota perspective.
- int num_tpl_nonlin_ineq_constraints () const

  Number of nonlinear inequality constraints from TPL perspective.
- Real **get_response_value_from_dakota** (const Response &resp) const

- template< typename VecT >
  void **get_nonlinear_ineq_constraints_from_dakota** (const Response &resp, VecT &values)
- template< typename VecT >
  void **get_best_nonlinear_ineq_constraints_from_tpl** (const VecT &values, RealVector &target)
- template< typename VecT >
  void **get_nonlinear_eq_constraints_from_dakota** (const Response &resp, VecT &values)
- template< typename VecT >
  void **get_best_nonlinear_eq_constraints_from_tpl** (const VecT &values, RealVector &target)

Protected Member Functions

- void configure_nonlinear_eq_adapters (NONLINEAR_EQUALITY_FORMAT, const Constraints &)
  Construct nonlinear equality maps needed to exchange data to/from Dakota and the TPL.
- void configure_nonlinear_ineq_adapters (NONLINEAR_INEQUALITY_FORMAT, const Constraints &, bool split_eqs)
  Construct nonlinear inequality maps needed to exchange data to/from Dakota and the TPL.

Protected Attributes

- int numDakotaObjectiveFns
  number of objective functions from Dakota perspective
- bool maxSense
  Single boolean (could be extended to multiple) indicating min/max sense of optimal value.
- int numDakotaNonlinearEqConstraints
  number of nonlinear equality constraints from Dakota perspective
- int numTPLNonlinearEqConstraints
  number of nonlinear equality constraints from TPL perspective
- std::vector< int > nonlinearEqConstraintMapIndices
  map from Dakota constraint number to TPL constraint number
- std::vector< double > nonlinearEqConstraintMapMultipliers
  multipliers for constraint transformations - may not be needed? - RWH
- std::vector< double > nonlinearEqConstraintTargets
  offsets for constraint transformations
- int numDakotaNonlinearIneqConstraints
  number of nonlinear inequality constraints from Dakota perspective
- int numTPLNonlinearIneqConstraints
  number of nonlinear inequality constraints actually used ... based conditionally on lower bounds using bigRealBoundSize and on whether TPL splits equalities into two inequalities
- std::vector< int > nonlinearIneqConstraintMapIndices
  map from Dakota constraint number to TPL constraint number
- std::vector< double > nonlinearIneqConstraintMapMultipliers
  multipliers for constraint transformations
- std::vector< double > nonlinearIneqConstraintMapShifts
  offsets for constraint transformations

14.289.1 Detailed Description

The TPLDataTransfer class provides ...

The documentation for this class was generated from the following files:

- DakotaTPLDataTransfer.hpp
- DakotaTPLDataTransfer.cpp

14.290 TrackerHTTP Class Reference

TrackerHTTP: a usage tracking module that uses HTTP/HTTPS via the curl library.

Classes

- struct Server

    struct to hold tracker/proxy pairs

Public Member Functions

- TrackerHTTP ()

    default constructor is allowed, but doesn't generate output
- TrackerHTTP (int world_rank=0)

    standard constructor with ProblemDescDB, rank
- ∼TrackerHTTP ()

    destructor to free handles
- void post_start (ProblemDescDB &problem_db)

    post the start of an analysis and archive start time
- void post_finish (unsigned runtime=0)

    post the completion of an analysis including elapsed time

Private Member Functions

- void initialize (int world_rank=0)

    shared initialization functions across constructors
- void url_add_field (std::string &url, const char ∗keyword, const std::string &value, bool delimit=true) const

    append keyword/value pair to url in GET style (with &keyword=value); set delimit = false to omit the &
- void build_default_data (std::string &url, std::time_t &rawtime, const std::string &mode) const

    construct URL with shared information for start/finish
- void send_data_using_get (const std::string &urltopost) const

    transmit data to the web server using GET
- void send_data_using_post (const std::string &datatopost)

    POST separate location and query; datatopost="name=daniel&project=curl".
- void split_string (const std::string &s, const char &delim, std::vector< std::string > &elems)

    Split a string on a delimiter and place tokens in elems.
- void parse_tracking_string (const std::string &dt)

    Populate serverList with tracker and proxy URLs from dt.
- void populate_method_list (ProblemDescDB &problem_db)

    extract list of methods from problem database
- std::string get_uid () const

    get the real user ID
- std::string get_username () const

    get the username as reported by the environment
- std::string get_hostname () const

    get the system hostname
- std::string get_os () const

    get the operating system
- std::string get_datetime (const std::time_t &rawtime) const

    get the date and time as a string YYYYMMDDHHMMSS

Private Attributes

- CURL * curlPtr

    pointer to the curl handler instance
- FILE * devNull

    pointer to /dev/null
- std::list< Server > serverList

    List of servers to try (tracker and proxy)
- long timeoutSeconds

    seconds until the request will timeout (may have issues with signals)
- std::string methodList

    list of active methods
- std::string dakotaVersion

    DAKOTA version.
- std::time_t startTime

    cached starting time in raw seconds
- short outputLevel

    verbosity control

14.290.1 Detailed Description

TrackerHTTP: a usage tracking module that uses HTTP/HTTPS via the curl library.

14.290.2 Member Function Documentation

14.290.2.1 void send_data_using_get (const std::string & *urltopost*) const [private]

transmit data to the web server using GET

whole url including location&fields

References TrackerHTTP::curlPtr, and TrackerHTTP::outputLevel.

14.290.2.2 void send_data_using_post (const std::string & *datatopost*) [private]

POST separate location and query; datatopost="name=daniel&project=curl".

separate location and query; datatopost="name=daniel&project=curl"

References TrackerHTTP::curlPtr, TrackerHTTP::outputLevel, and TrackerHTTP::serverList.

Referenced by TrackerHTTP::post_finish(), and TrackerHTTP::post_start().

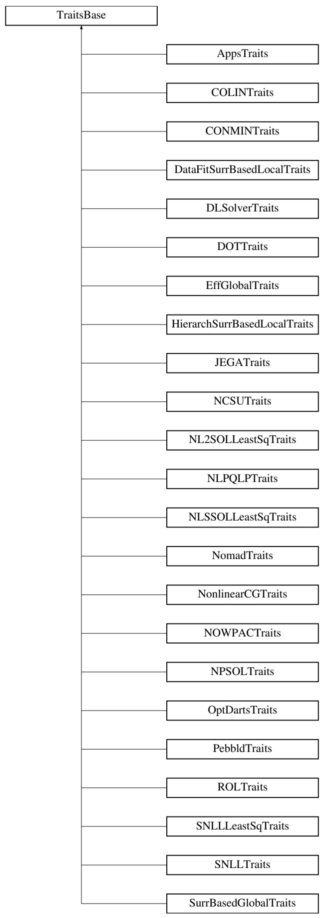
The documentation for this class was generated from the following files:

- TrackerHTTP.hpp
- TrackerHTTP.cpp

14.291 TraitsBase Class Reference

Base class for traits.

Inheritance diagram for TraitsBase:



Public Member Functions

- TraitsBase ()

    default constructor
- virtual ∼TraitsBase ()

    destructor
- virtual bool is_derived ()

    A temporary query used in the refactor.
- virtual bool requires_bounds ()

    Return the flag indicating whether method requires bounds.
- virtual bool supports_linear_equality ()

    Return the flag indicating whether method supports linear equalities.
- virtual bool supports_linear_inequality ()

    Return the flag indicating whether method supports linear inequalities.
- virtual LINEAR_INEQUALITY_FORMAT linear_inequality_format ()

    Return the format used for linear inequality constraints.
- virtual bool supports_nonlinear_equality ()

    Return the flag indicating whether method supports nonlinear equalities.
- virtual NONLINEAR_EQUALITY_FORMAT nonlinear_equality_format ()

    Return the format used for nonlinear equality constraints.
- virtual bool supports_nonlinear_inequality ()

    Return the flag indicating whether method supports nonlinear inequalities.
- virtual NONLINEAR_INEQUALITY_FORMAT nonlinear_inequality_format ()

    Return the format used for nonlinear inequality constraints.

- virtual bool expects_nonlinear_inequalities_first ()

    Return the flag indicating whether method expects nonlinear inequality constraints followed by nonlinear equality constraints.
- virtual bool supports_scaling ()

    Return the flag indicating whether method supports parameter scaling.
- virtual bool supports_least_squares ()

    Return the flag indicating whether method supports least squares.
- virtual bool supports_multiobjectives ()

    Return flag indicating whether method supports multiobjective optimization.
- virtual bool supports_continuous_variables ()

    Return the flag indicating whether method supports continuous variables.
- virtual bool supports_discrete_variables ()

    Return the flag indicating whether method supports continuous variables.
- virtual bool provides_best_objective ()

    Return the flag indicating whether method provides best objective result.
- virtual bool provides_best_parameters ()

    Return the flag indicating whether method provides best parameters result.
- virtual bool provides_best_constraint ()

    Return the flag indicating whether method provides best constraint result.
- virtual bool provides_final_gradient ()

    Return the flag indicating whether method provides final gradient result.
- virtual bool provides_final_hessian ()

    Return the flag indicating whether method provides final hessian result.

14.291.1 Detailed Description

Base class for traits.

TraitsBase provides default traits through various accessors .

The documentation for this class was generated from the following files:

- DakotaTraitsBase.hpp
- DakotaTraitsBase.cpp

14.292 UsageTracker Class Reference

Lightweight class to manage conditionally active Curl-based HTTP tracker via PIMPL.

Public Member Functions

- UsageTracker ()

    default construction: no output
- UsageTracker (int world_rank)

    standard constructor; will output on rank 0
- void post_start (ProblemDescDB &problem_db)

    post the start of an analysis and archive start time
- void post_finish (unsigned runtime=0)

    post the completion of an analysis including elapsed time

Private Member Functions

- UsageTracker (const UsageTracker &)
  copy construction is disallowed

Private Attributes

- std::shared_ptr< TrackerHTTP > pTrackerHTTP
  posts usage data to Web server; using shared_ptr due to potentially incomplete type and requirements for checked_delete in debug builds (scoped_ptr would suffice)

14.292.1 Detailed Description

Lightweight class to manage conditionally active Curl-based HTTP tracker via PIMPL.

All conditional compilation in managed in the cpp file; all operations are no-op in this wrapper if not enabling tracking...

14.292.2 Constructor & Destructor Documentation

14.292.2.1 UsageTracker (int *world_rank*)

standard constructor; will output on rank 0

standard constructor; will output on rank 0 and only initializes if tracking compiled in and not disable by environment

References UsageTracker::pTrackerHTTP.

The documentation for this class was generated from the following files:

- UsageTracker.hpp
- UsageTracker.cpp

14.293 Var_icheck Struct Reference

structure for verifying bounds and initial point for string-valued vars

Public Attributes

- const char ∗ **name**
- size_t DataVariablesRep::∗ **n**
- void(∗ **vgen**)(DataVariablesRep ∗, size_t)
- IntVector DataVariablesRep::∗ **L**
- IntVector DataVariablesRep::∗ **U**
- IntVector DataVariablesRep::∗ **V**
- StringArray DataVariablesRep::∗ **Lbl**

14.293.1 Detailed Description

structure for verifying bounds and initial point for string-valued vars

structure for verifying bounds and initial point for integer-valued vars

The documentation for this struct was generated from the following file:

- NIDRProblemDescDB.cpp

14.294 Var_rcheck Struct Reference

structure for verifying bounds and initial point for real-valued vars

Public Attributes

- const char ∗ **name**
- size_t DataVariablesRep::∗ **n**
- void(∗ **vgen**)(DataVariablesRep ∗, size_t)
- RealVector DataVariablesRep::∗ **L**
- RealVector DataVariablesRep::∗ **U**
- RealVector DataVariablesRep::∗ **V**
- StringArray DataVariablesRep::∗ **Lbl**

14.294.1 Detailed Description

structure for verifying bounds and initial point for real-valued vars

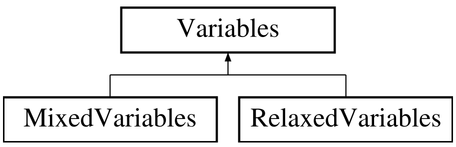
The documentation for this struct was generated from the following file:

- NIDRProblemDescDB.cpp

14.295 Variables Class Reference

Base class for the variables class hierarchy.

Inheritance diagram for Variables:



Public Member Functions

- Variables ()

  default constructor
- Variables (const ProblemDescDB &problem_db)

  standard constructor (explicit disallows its use for implicit type conversion)
- Variables (const SharedVariablesData &svd)

  alternate constructor for instantiations on the fly (explicit disallows its use for implicit type conversion)
- Variables (const Variables &vars)

  copy constructor
- virtual ∼Variables ()

  destructor
- Variables operator= (const Variables &vars)

  assignment operator
- virtual void read (std::istream &s)

  read a variables object from an std::istream
- virtual void write (std::ostream &s, unsigned short vars_part=ALL_VARS) const

write a variables object to an std::ostream, e.g., the console, optionally specifying which partition (all/active/inactive)
- virtual void write_aprepro (std::ostream &s) const

  write a variables object to an std::ostream in aprepro format, e.g., a parameters file
- virtual void read_annotated (std::istream &s)

  read a variables object in annotated format from an istream
- virtual void write_annotated (std::ostream &s) const

  write a variables object in annotated format to an std::ostream
- virtual void read_tabular (std::istream &s, unsigned short vars_part=ALL_VARS)

  read a variables object in tabular format from an istream, optionally specifying which partition (all/active/inactive)
- virtual void write_tabular (std::ostream &s, unsigned short vars_part=ALL_VARS) const

  write a variables object in tabular format to an std::ostream, optionally specifying which partition (all/active/inactive)
- virtual void write_tabular_partial (std::ostream &s, size_t start_index, size_t num_items) const

  write range of variables in tabular format to an std::ostream
- virtual void write_tabular_labels (std::ostream &s, unsigned short vars_part=ALL_VARS) const

  write the labels in input spec order to a std::ostream, optionally specifying which partition (all/active/inactive)
- virtual void write_tabular_partial_labels (std::ostream &s, size_t start_index, size_t num_items) const

  write range of variable labels in input spec order to a std::ostream
- virtual void read (MPIUnpackBuffer &s)

  read a variables object from a packed MPI buffer
- virtual void write (MPIPackBuffer &s) const

  write a variables object to a packed MPI buffer
- size_t tv () const

  total number of vars
- size_t total_active () const

  total number of active vars
- size_t cv () const

  number of active continuous vars
- size_t cv_start () const

  start index of active continuous vars
- size_t div () const

  number of active discrete int vars
- size_t div_start () const

  start index of active discrete int vars
- size_t dsv () const

  number of active discrete string vars
- size_t dsv_start () const

  start index of active discrete string vars
- size_t drv () const

  number of active discrete real vars
- size_t drv_start () const

  start index of active discrete real vars
- size_t icv () const

  number of inactive continuous vars
- size_t icv_start () const

  start index of inactive continuous vars
- size_t idiv () const

  number of inactive discrete int vars
- size_t idiv_start () const

  start index of inactive discrete int vars
- size_t idsv () const

  number of inactive discrete string vars

- size_t idsv_start () const
  start index of inactive discrete string vars
- size_t idrv () const
  number of inactive discrete real vars
- size_t idrv_start () const
  start index of inactive discrete real vars
- size_t acv () const
  total number of continuous vars
- size_t adiv () const
  total number of discrete integer vars
- size_t adsv () const
  total number of discrete string vars
- size_t adrv () const
  total number of discrete real vars
- const SharedVariablesData & shared_data () const
  return sharedVarsData
- SharedVariablesData & shared_data ()
  return sharedVarsData
- void shape ()
  shape a Variables object based on sharedVarsData
- void reshape ()
  reshape an existing Variables object based on updated sharedVarsData
- Real continuous_variable (size_t index) const
  return an active continuous variable
- const RealVector & continuous_variables () const
  return the active continuous variables (Note: returns a view by const reference, but initializing a RealVector from this reference invokes the Teuchos matrix copy constructor to create a Teuchos::Copy instance; to obtain a mutable view, use continuous_variables_view())
- void continuous_variable (Real c_var, size_t index)
  set an active continuous variable
- void continuous_variables (const RealVector &c_vars)
  set the active continuous variables
- int discrete_int_variable (size_t index) const
  return an active discrete integer variable
- const IntVector & discrete_int_variables () const
  return the active discrete integer variables (Note: returns a view by const reference, but initializing an IntVector from this reference invokes the Teuchos matrix copy constructor to create a Teuchos::Copy instance; to obtain a mutable view, use discrete_int_variables_view())
- void discrete_int_variable (int di_var, size_t index)
  set an active discrete integer variable
- void discrete_int_variables (const IntVector &di_vars)
  set the active discrete integer variables
- const String & discrete_string_variable (size_t index) const
  return an active discrete string variable
- StringMultiArrayConstView discrete_string_variables () const
  return the active discrete string variables (Note: returns a view by const reference, but initializing a StringArray from this reference invokes the Teuchos matrix copy constructor to create a Teuchos::Copy instance; to obtain a mutable view, use discrete_string_variables_view())
- void discrete_string_variable (const String &ds_var, size_t index)
  set an active discrete string variable
- void discrete_string_variables (StringMultiArrayConstView ds_vars)
  set the active discrete string variables

- Real discrete_real_variable (size_t index) const

    return an active discrete real variable

- const RealVector & discrete_real_variables () const

    return the active discrete real variables (Note: returns a view by const reference, but initializing a RealVector from this reference invokes the Teuchos matrix copy constructor to create a Teuchos::Copy instance; to obtain a mutable view, use discrete_real_variables_view())

- void discrete_real_variable (Real dr_var, size_t index)

    set an active discrete real variable

- void discrete_real_variables (const RealVector &dr_vars)

    set the active discrete real variables

- void active_variables (const Variables &vars)

    copy the active cv/div/dsv/drv variables from vars

- void inactive_variables (const Variables &vars)

    copy the inactive cv/div/dsv/drv variables from vars

- void all_variables (const Variables &vars)

    copy all cv/div/dsv/drv variables from vars

- void inactive_from_active (const Variables &vars)

    copy the active cv/div/dsv/drv variables from vars to inactive on this

- RealVector & continuous_variables_view ()

    return a mutable view of the active continuous variables

- IntVector & discrete_int_variables_view ()

    return a mutable view of the active discrete integer variables

- StringMultiArrayView discrete_string_variables_view ()

    return a mutable view of the active discrete string variables

- RealVector & discrete_real_variables_view ()

    return a mutable view of the active discrete real variables

- StringMultiArrayConstView continuous_variable_labels () const

    return the active continuous variable labels

- void continuous_variable_labels (StringMultiArrayConstView cv_labels)

    set the active continuous variable labels

- void continuous_variable_label (const String &cv_label, size_t index)

    set an active continuous variable label

- StringMultiArrayConstView discrete_int_variable_labels () const

    return the active discrete integer variable labels

- void discrete_int_variable_labels (StringMultiArrayConstView div_labels)

    set the active discrete integer variable labels

- void discrete_int_variable_label (const String &div_label, size_t index)

    set an active discrete integer variable label

- StringMultiArrayConstView discrete_string_variable_labels () const

    return the active discrete string variable labels

- void discrete_string_variable_labels (StringMultiArrayConstView dsv_labels)

    set the active discrete string variable labels

- void discrete_string_variable_label (const String &dsv_label, size_t index)

    set an active discrete string variable label

- StringMultiArrayConstView discrete_real_variable_labels () const

    return the active discrete real variable labels

- void discrete_real_variable_labels (StringMultiArrayConstView drv_labels)

    set the active discrete real variable labels

- void discrete_real_variable_label (const String &drv_label, size_t index)

    set an active discrete real variable label

- UShortMultiArrayConstView continuous_variable_types () const

return the active continuous variable types
- void continuous_variable_types (UShortMultiArrayConstView cv_types)

  set the active continuous variable types
- void continuous_variable_type (unsigned short cv_type, size_t index)

  set an active continuous variable type
- UShortMultiArrayConstView discrete_int_variable_types () const

  return the active discrete integer variable types
- void discrete_int_variable_types (UShortMultiArrayConstView div_types)

  set the active discrete integer variable types
- void discrete_int_variable_type (unsigned short div_type, size_t index)

  set an active discrete integer variable type
- UShortMultiArrayConstView discrete_string_variable_types () const

  return the active discrete string variable types
- void discrete_string_variable_types (UShortMultiArrayConstView dsv_types)

  set the active discrete string variable types
- void discrete_string_variable_type (unsigned short dsv_type, size_t index)

  set an active discrete string variable type
- UShortMultiArrayConstView discrete_real_variable_types () const

  return the active discrete real variable types
- void discrete_real_variable_types (UShortMultiArrayConstView drv_types)

  set the active discrete real variable types
- void discrete_real_variable_type (unsigned short drv_type, size_t index)

  set an active discrete real variable type
- SizetMultiArrayConstView continuous_variable_ids () const

  return the active continuous variable position identifiers
- void continuous_variable_ids (SizetMultiArrayConstView cv_ids)

  set the active continuous variable position identifiers
- void continuous_variable_id (size_t cv_id, size_t index)

  set an active continuous variable position identifier
- const RealVector & inactive_continuous_variables () const

  return the inactive continuous variables
- void inactive_continuous_variables (const RealVector &ic_vars)

  set the inactive continuous variables
- void inactive_continuous_variable (Real ic_var, size_t index)

  set an inactive continuous variable
- const IntVector & inactive_discrete_int_variables () const

  return the inactive discrete int variables
- void inactive_discrete_int_variables (const IntVector &idi_vars)

  set the inactive discrete int variables
- void inactive_discrete_int_variable (int idi_var, size_t index)

  set an inactive discrete int variable
- StringMultiArrayConstView inactive_discrete_string_variables () const

  return the inactive discrete string variables
- void inactive_discrete_string_variables (StringMultiArrayConstView ids_vars)

  set the inactive discrete string variables
- void inactive_discrete_string_variable (const String &ids_var, size_t index)

  set an inactive discrete string variable
- const RealVector & inactive_discrete_real_variables () const

  return the inactive discrete real variables
- void inactive_discrete_real_variables (const RealVector &idr_vars)

  set the inactive discrete real variables

- void inactive_discrete_real_variable (Real idr_var, size_t index)
  set an inactive discrete real variable
- StringMultiArrayConstView inactive_continuous_variable_labels () const
  return the inactive continuous variable labels
- void inactive_continuous_variable_labels (StringMultiArrayConstView ic_vars)
  set the inactive continuous variable labels
- StringMultiArrayConstView inactive_discrete_int_variable_labels () const
  return the inactive discrete variable labels
- void inactive_discrete_int_variable_labels (StringMultiArrayConstView idi_vars)
  set the inactive discrete variable labels
- StringMultiArrayConstView inactive_discrete_string_variable_labels () const
  return the inactive discrete variable labels
- void inactive_discrete_string_variable_labels (StringMultiArrayConstView ids_vars)
  set the inactive discrete variable labels
- StringMultiArrayConstView inactive_discrete_real_variable_labels () const
  return the inactive discrete variable labels
- void inactive_discrete_real_variable_labels (StringMultiArrayConstView idr_vars)
  set the inactive discrete variable labels
- UShortMultiArrayConstView inactive_continuous_variable_types () const
  return the inactive continuous variable types
- UShortMultiArrayConstView inactive_discrete_int_variable_types () const
  return the inactive discrete integer variable types
- UShortMultiArrayConstView inactive_discrete_string_variable_types () const
  return the inactive discrete string variable types
- UShortMultiArrayConstView inactive_discrete_real_variable_types () const
  return the inactive discrete real variable types
- SizetMultiArrayConstView inactive_continuous_variable_ids () const
  return the inactive continuous variable position identifiers
- const RealVector & all_continuous_variables () const
  returns a single array with all continuous variables
- void all_continuous_variables (const RealVector &ac_vars)
  sets all continuous variables using a single array
- void all_continuous_variable (Real ac_var, size_t index)
  set a variable within the all continuous array
- const IntVector & all_discrete_int_variables () const
  returns a single array with all discrete variables
- void all_discrete_int_variables (const IntVector &adi_vars)
  sets all discrete variables using a single array
- void all_discrete_int_variable (int adi_var, size_t index)
  set a variable within the all discrete array
- StringMultiArrayConstView all_discrete_string_variables () const
  returns a single array with all discrete variables
- void all_discrete_string_variables (StringMultiArrayConstView ads_vars)
  sets all discrete variables using a single array
- void all_discrete_string_variable (const String &ads_var, size_t index)
  set a variable within the all discrete array
- const RealVector & all_discrete_real_variables () const
  returns a single array with all discrete variables
- void all_discrete_real_variables (const RealVector &adr_vars)
  sets all discrete variables using a single array
- void all_discrete_real_variable (Real adr_var, size_t index)

set a variable within the all discrete array
- void as_vector (const StringSetArray &dss_vals, RealVector &var_values) const
  get the active variables as a vector of reals, converting string values to zero-based set indices
- StringMultiArrayView all_continuous_variable_labels () const
  returns a single array with all continuous variable labels
- void all_continuous_variable_labels (StringMultiArrayConstView acv_labels)
  sets all continuous variable labels using a single array
- void all_continuous_variable_label (const String &acv_label, size_t index)
  set a label within the all continuous label array
- StringMultiArrayView all_discrete_int_variable_labels () const
  returns a single array with all discrete variable labels
- void all_discrete_int_variable_labels (StringMultiArrayConstView adiv_labels)
  sets all discrete variable labels using a single array
- void all_discrete_int_variable_label (const String &adiv_label, size_t index)
  set a label within the all discrete label array
- StringMultiArrayView all_discrete_string_variable_labels () const
  returns a single array with all discrete variable labels
- void all_discrete_string_variable_labels (StringMultiArrayConstView adsv_labels)
  sets all discrete variable labels using a single array
- void all_discrete_string_variable_label (const String &adsv_label, size_t index)
  set a label within the all discrete label array
- StringMultiArrayView all_discrete_real_variable_labels () const
  returns a single array with all discrete variable labels
- void all_discrete_real_variable_labels (StringMultiArrayConstView adrv_labels)
  sets all discrete variable labels using a single array
- void all_discrete_real_variable_label (const String &adrv_label, size_t index)
  set a label within the all discrete label array
- UShortMultiArrayConstView all_continuous_variable_types () const
  return all continuous variable types
- UShortMultiArrayConstView all_discrete_int_variable_types () const
  return all discrete variable types
- UShortMultiArrayConstView all_discrete_string_variable_types () const
  return all discrete variable types
- UShortMultiArrayConstView all_discrete_real_variable_types () const
  return all discrete variable types
- SizetMultiArrayConstView all_continuous_variable_ids () const
  return all continuous variable position identifiers
- SizetMultiArrayConstView all_discrete_int_variable_ids () const
  return all discrete integer variable position identifiers
- SizetMultiArrayConstView all_discrete_string_variable_ids () const
  return all discrete string variable position identifiers
- SizetMultiArrayConstView all_discrete_real_variable_ids () const
  return all discrete real variable position identifiers
- StringArray ordered_labels (unsigned short vars_part=ALL_VARS) const
  get all or active labels in input spec order
- Variables copy (bool deep_svd=false) const
  a deep variables copy for use in history mechanisms (SharedVariablesData uses a shallow copy by default)
- const std::pair< short, short > & view () const
  returns variablesView
- std::pair< short, short > get_view (const ProblemDescDB &problem_db) const
  defines variablesView from problem_db attributes

- void inactive_view (short view2)

    sets the inactive view based on higher level (nested) context
- const String & variables_id () const

    returns the variables identifier string
- const SizetArray & variables_components_totals () const

    returns the number of variables for each of the constitutive components
- bool is_null () const

    function to check variablesRep (does this envelope contain a letter)

Protected Member Functions

- Variables (BaseConstructor, const ProblemDescDB &problem_db, const std::pair< short, short > &view)

    constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- Variables (BaseConstructor, const SharedVariablesData &svd)

    constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139)
- void build_views ()

    construct active/inactive views of all variables arrays
- void build_active_views ()

    construct active views of all variables arrays
- void build_inactive_views ()

    construct inactive views of all variables arrays

Protected Attributes

- SharedVariablesData sharedVarsData

    reference-counted instance of shared variables data: id's, labels, counts
- RealVector allContinuousVars

    array combining all of the continuous variables
- IntVector allDiscreteIntVars

    array combining all of the discrete integer variables
- StringMultiArray allDiscreteStringVars

    array combining all of the discrete string variables
- RealVector allDiscreteRealVars

    array combining all of the discrete real variables
- RealVector continuousVars

    the active continuous variables array view
- IntVector discreteIntVars

    the active discrete integer variables array view
- RealVector discreteRealVars

    the active discrete real variables array view
- RealVector inactiveContinuousVars

    the inactive continuous variables array view
- IntVector inactiveDiscreteIntVars

    the inactive discrete integer variables array view
- RealVector inactiveDiscreteRealVars

    the inactive discrete real variables array view

Private Member Functions

- std::shared_ptr< Variables > get_variables (const ProblemDescDB &problem_db)

  Used by the standard envelope constructor to instantiate the correct letter class.
- std::shared_ptr< Variables > get_variables (const SharedVariablesData &svd) const

  Used by the alternate envelope constructors, by read functions, and by copy() to instantiate a new letter class.
- short method_map (short view_spec, bool relaxed) const

  infer domain from method selection
- short method_domain (const ProblemDescDB &problem_db) const

  infer domain from method selection
- short method_view (const ProblemDescDB &problem_db) const

  infer view from method selection
- short response_view (const ProblemDescDB &problem_db) const

  infer view from type of response data set
- void check_view_compatibility ()

  perform sanity checks on view.first and view.second after update
- template<class Archive >
  void load (Archive &ar, const unsigned int version)

  read a Variables object from an archive
- template<class Archive >
  void save (Archive &ar, const unsigned int version) const

  write a Variables object to an archive

Friends

- class boost::serialization::access

  for serializing private data members
- bool operator== (const Variables &vars1, const Variables &vars2)

  strict equality operator (for boost hash-based lookups)
- bool operator!= (const Variables &vars1, const Variables &vars2)

  strict inequality operator
- bool nearby (const Variables &vars1, const Variables &vars2, Real rel_tol)

  tolerance-based equality operator
- std::size_t hash_value (const Variables &vars)

  hash_value

14.295.1 Detailed Description

Base class for the variables class hierarchy.

The Variables class is the base class for the class hierarchy providing design, uncertain, and state variables for continuous and discrete domains within a Model. Using the fundamental arrays from the input specification, different derived classes define different views of the data. For memory efficiency and enhanced polymorphism, the variables hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (Variables) serves as the envelope and one of the derived classes (selected in Variables::get_variables()) serves as the letter.

14.295.2 Member Function Documentation

14.295.2.1 StringMultiArrayView discrete_string_variables_view ( ) [inline]

return a mutable view of the active discrete string variables

same as discrete_string_variables(), except mutable view

References Variables::allDiscreteStringVars, SharedVariablesData::dsv(), SharedVariablesData::dsv_start(), and Variables::sharedVarsData.

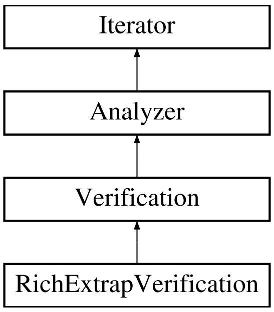
The documentation for this class was generated from the following file:

- DakotaVariables.hpp

14.296 Verification Class Reference

Base class for managing common aspects of verification studies.

Inheritance diagram for Verification:



Public Member Functions

- bool resize ()
  reinitializes iterator based on new variable size

Protected Member Functions

- Verification (ProblemDescDB &problem_db, Model &model)
  constructor
- Verification (unsigned short method_name, Model &model)
  alternate constructor for instantiations "on the fly"
- ∼Verification ()
  destructor
- void print_results (std::ostream &s, short results_state=FINAL_RESULTS)
  print the final iterator results

Additional Inherited Members

14.296.1 Detailed Description

Base class for managing common aspects of verification studies.

The Verification base class manages common data and functions, such as those involving ...

14.296.2 Member Function Documentation

14.296.2.1 void print_results (std::ostream & *s*, short *results_state* = FINAL_RESULTS) [protected], [virtual]

print the final iterator results

This virtual function provides additional iterator-specific final results outputs beyond the function evaluation summary printed in finalize_run().

Reimplemented from Analyzer.

Reimplemented in RichExtrapVerification.

References Analyzer::print_results().

Referenced by RichExtrapVerification::print_results().

The documentation for this class was generated from the following files:

- DakotaVerification.hpp
- DakotaVerification.cpp

14.297 VLint Struct Reference

structure for validating integer uncertain variable labels, bounds, values

Public Attributes

- int **n**
- VarLabel Var_Info::∗ **VL**
- Var_uinfo ∗ **vui**
- StringArray DataVariablesRep::∗ **Labels**
- IntVector DataVariablesRep::∗ **LowerBnds**
- IntVector DataVariablesRep::∗ **UpperBnds**
- IntVector DataVariablesRep::∗ **UncVars**

14.297.1 Detailed Description

structure for validating integer uncertain variable labels, bounds, values

The documentation for this struct was generated from the following file:

- NIDRProblemDescDB.cpp

14.298 VLreal Struct Reference

structure for validating real uncertain variable labels, bounds, values

Public Attributes

- int **n**
- VarLabel Var_Info::∗ **VL**
- Var_uinfo ∗ **vui**
- StringArray DataVariablesRep::∗ **Labels**

- RealVector DataVariablesRep::∗ **LowerBnds**
- RealVector DataVariablesRep::∗ **UpperBnds**
- RealVector DataVariablesRep::∗ **UncVars**

14.298.1 Detailed Description

structure for validating real uncertain variable labels, bounds, values

The documentation for this struct was generated from the following file:

- NIDRProblemDescDB.cpp

14.299 VLstr Struct Reference

structure for validating string uncertain variable labels, bounds, values

Public Attributes

- int **n**
- VarLabel Var_Info::∗ **VL**
- Var_uinfo ∗ **vui**
- StringArray DataVariablesRep::∗ **Labels**
- StringArray DataVariablesRep::∗ **LowerBnds**
- StringArray DataVariablesRep::∗ **UpperBnds**
- StringArray DataVariablesRep::∗ **UncVars**

14.299.1 Detailed Description

structure for validating string uncertain variable labels, bounds, values

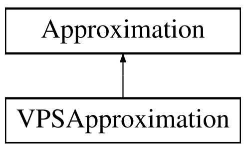
The documentation for this struct was generated from the following file:

- NIDRProblemDescDB.cpp

14.300 VPSApproximation Class Reference

Derived approximation class for VPS implementation.

Inheritance diagram for VPSApproximation:



Public Member Functions

- VPSApproximation ()

  default constructor

- VPSApproximation (const ProblemDescDB &problem_db, const SharedApproxData &shared_data, const String &approx_label)

    standard constructor (to call VPS from an input deck)
- VPSApproximation (const SharedApproxData &shared_data)

    Alternate constructor (to call VPS from another method like POF-darts)
- ∼VPSApproximation ()

    destructor
- bool **VPS_execute** ()
- void **VPS_create_containers** ()
- void **VPS_retrieve_neighbors** (size_t ipoint, bool update_point_neighbors)
- void **VPS_adjust_extend_neighbors_of_all_points** ()
- void **VPS_extend_neighbors** (size_t ipoint)
- void **VPS_build_local_surrogate** (size_t cell_index)
- double **VPS_evaluate_surrogate** (double ∗x)
- void **VPS_destroy_global_containers** ()
- void **retrieve_permutations** (size_t &m, size_t ∗∗&perm, size_t num_dim, size_t upper_bound, bool force_-sum_constraint, size_t sum_constraint)
- void **build_radial_basis_function** (size_t icell)
- void **VPS_LS_retrieve_weights** (size_t cell_index)
- double **evaluate_basis_function** (double ∗x, size_t icell, size_t ibasis)
- int **constrained_LeastSquare** (size_t n, size_t m, double ∗∗H, double ∗w, double ∗f)
- double **vec_dot_vec** (size_t n, double ∗vec_a, double ∗vec_b)
- double **vec_pow_vec** (size_t num_dim, double ∗vec_a, size_t ∗vec_b)
- bool **Cholesky** (int n, double ∗∗A, double ∗∗LD)
- void **Cholesky_solver** (int n, double ∗∗LD, double ∗b, double ∗x)
- void **GMRES** (size_t n, double ∗∗A, double ∗b, double ∗x, double eps)
- void **printMatrix** (size_t m, size_t n, double ∗∗M)
- void **initiate_random_number_generator** (unsigned long x)
- double **generate_a_random_number** ()
- size_t **retrieve_closest_cell** (double ∗x)
- bool **trim_line_using_Hyperplane** (size_t num_dim, double ∗st, double ∗end, double ∗qH, double ∗nH)
- double **f_test** (double ∗x)
- double ∗ **grad_f_test** (double ∗x)
- double ∗∗ **hessian_f_test** (double ∗x)
- void **generate_poisson_disk_sample** (double r)
- void **generate_MC_sample** ()
- void **isocontouring** (std::string file_name, bool plot_test_function, bool plot_surrogate, std::vector< double > contours)
- void **isocontouring_solid** (std::string file_name, bool plot_test_function, bool plot_surrogate, std::vector< double > contours)
- void **plot_neighbors** ()

Protected Member Functions

- int min_coefficients () const

    return the minimum number of samples (unknowns) required to build the derived class approximation type in numVars dimensions
- void build ()

    builds the approximation from scratch
- Real value (const Variables &vars)

    retrieve the predicted function value for a given parameter set
- const RealVector & gradient (const Variables &vars)

    retrieve the function gradient at the predicted value for a given parameter set
- Real prediction_variance (const Variables &vars)

    retrieve the variance of the predicted value for a given parameter set

Private Types

- enum **subsurrogate** { **LS**, **GP** }
- enum **subsurrogate_basis** { **polynomial**, **radial** }
- enum **testfunction** {
  SmoothHerbie, **Herbie**, **Cone**, **Cross**,
  UnitSphere, **Linear34** }

Private Member Functions

- void VPSmodel_build ()

  Function to compute coefficients governing the VPS surrogates.
- void VPSmodel_apply (const RealVector &new_x, bool variance_flag, bool gradients_flag)

  Function returns a response value using the VPS surface.

Private Attributes

- Real approxValue

  value of the approximation returned by value()
- Real approxVariance

  value of the approximation returned by prediction_variance()
- RealMatrix trainPoints

  A 2-D array (num sample sites = rows, num vars = columns) used to create the Gaussian process.
- RealMatrix trainValues

  An array of response values; one response value per sample site.
- size_t numObs

  The number of observations on which the GP surface is built.
- int surrogateOrder

  The order of the polynomial in each Voronoi cell.
- subsurrogate **_vps_subsurrogate**
- subsurrogate_basis **_vps_subsurrogate_basis**
- testfunction **_vps_test_function**
- double **Q** [1220]
- int **indx**
- double **cc**
- double **c**
- double **zc**
- double **zx**
- double **zy**
- size_t **qlen**
- size_t **_n_dim**
- double ∗ **_xmin**
- double ∗ **_xmax**
- double **_diag**
- size_t **_num_inserted_points**
- double ∗∗ **_sample_points**
- double ∗ **_fval**
- double ∗∗ **_fgrad**
- double ∗∗∗ **_fhess**
- size_t ∗∗ **_sample_neighbors**
- size_t ∗∗ **_vps_ext_neighbors**
- size_t **_vps_order**
- size_t **_num_GMRES**

- size_t ∗ **_num_cell_basis_functions**
- double ∗ **_sample_vsize**
- double ∗ **_vps_dfar**
- double ∗∗∗ **_sample_basis**
- double **_max_vsize**
- double **_disc_min_jump**
- double **_disc_min_grad**
- double **_f_min**
- double **_f_max**
- size_t ∗∗∗ **_vps_t**
- double ∗∗ **_vps_w**
- SharedApproxData **sharedData**
- std::vector< Approximation > **gpApproximations**
- Variables **gpEvalVars**
- bool **_use_derivatives**
- bool **_use_gradient**
- bool **_use_hessian**

Static Private Attributes

- static VPSApproximation ∗ VPSinstance
  pointer to the active object instance used within the static evaluator

Additional Inherited Members

14.300.1 Detailed Description

Derived approximation class for VPS implementation.

```
The VPSApproximation class provides a set of piecewise surrogate approximations
```

each of which is valid within a Voronoi cell.

14.300.2 Member Function Documentation

14.300.2.1 void VPSmodel_apply (const RealVector & *new_x*, bool *variance_flag*, bool *gradients_flag*) [private]

Function returns a response value using the VPS surface.

The response value is computed at the design point specified by the RealVector function argument.

References VPSApproximation::approxValue.

Referenced by VPSApproximation::gradient(), VPSApproximation::prediction_variance(), and VPSApproximation::value().

14.300.3 Member Data Documentation

14.300.3.1 VPSApproximation ∗ VPSinstance [static], [private]

pointer to the active object instance used within the static evaluator

default constructor

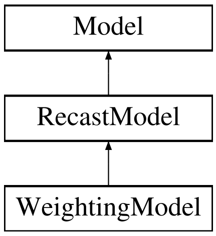
The documentation for this class was generated from the following files:

- VPSApproximation.hpp
- VPSApproximation.cpp

14.301 WeightingModel Class Reference

Weighting specialization of RecastModel.

Inheritance diagram for WeightingModel:



Public Member Functions

- WeightingModel (Model &sub_model)

  standard constructor
- ∼WeightingModel ()

  destructor

Protected Member Functions

- void assign_instance ()

  assign static pointer instance to this for use in static transformation functions
- void init_metadata () override

  default clear metadata in Recasts; derived classes can override to no-op

Static Protected Member Functions

- static void **primary_resp_weighter** (const Variables &sub_model_vars, const Variables &recast_vars, const Response &sub_model_response, Response &weighted_response)
- static void **primary_resp_unweighter** (const Variables &recast_vars, const Variables &sub_model_vars, const Response &weighted_resp, Response &unweighted_resp)=delete

Static Private Attributes

- static WeightingModel ∗ weightModelInstance

  static pointer to this class for use in static callbacks

Additional Inherited Members

14.301.1 Detailed Description

Weighting specialization of RecastModel.

Specialization of a RecastModel that manages Response weighting (could be implemented as special case of ScalingModel, but kept separate for simplicity for now). This class provides a simple constructor that forwards to the more complicated RecastModel API

14.301.2 Member Data Documentation

14.301.2.1 WeightingModel * weightModelInstance [static], [private]

static pointer to this class for use in static callbacks

initialization of static needed by RecastModel

Referenced by WeightingModel::assign_instance().

The documentation for this class was generated from the following files:

- WeightingModel.hpp
- WeightingModel.cpp

14.302 WorkdirHelper Class Reference

Static Public Member Functions

- static void initialize ()
  initialize (at runtime) cached values for paths and environment
- static const std::string & startup_pwd ()
  Query for dakota's startup $PWD.
- static void change_directory (const bfs::path &new_dir)
  change current directory
- static void prepend_preferred_env_path (const std::string &extra_path)
  Prepend cached preferredEnvPath with extra_path and update $PATH environment variable.
- static void set_environment (const std::string &env_name, const std::string &env_val, bool overwrite_-flag=true)
  Set an environment variable.
- static bfs::path which (const std::string &driver_name)
  Returns the bfs::path for the analysis driver, supporting typical windows filename extensions, or empty if not found.
- static bfs::path rel_to_abs (const bfs::path &subdir_path)
  get a valid absolute bfs::path to a subdirectory relative to rundir
- static StringArray tokenize_driver (const String &user_an_driver)
  tokenize a white-space separated analysis driver, respecting escapes and nested quotes
- static bool resolve_driver_path (String &an_driver)
  parse off the first whitespace-separated entry in the user's analysis_driver, and convert it to an absolute path if it begins with ./ or ../, replacing the passed string if needed. Returns true if the first token was modified.
- static void split_wildcard (const std::string &path_with_wc, bfs::path &search_dir, bfs::path &wild_card)
  given a string with an optional path and a wildcard, e.g., /tmp/D.?pp, parse it into the search path /tmp (default .) and the wildcard D*.?pp. Return wild_card as path to reduce wstring conversions*
- static bfs::path concat_path (const bfs::path &p_in, const String &tag)
  concatenate a string onto the end of a path
- static bfs::path system_tmp_file (const std::string &prefix)
  generate a valid temporary file name prefix_%%%%%%%%
- static bfs::path system_tmp_path ()
  get the system tmp path, e.g., /tmp or C:\temp
- static bool create_directory (const bfs::path &dir_path, short mkdir_option)
  Create a directory, with options for remove or error.
- static void recursive_remove (const bfs::path &rm_path, short fileop_option)
  Remove a path (file, directory, or symlink) without regard to its type. Only error if existed and there's an error in the remove.

- static void rename (const bfs::path &old_path, const bfs::path &new_path, short fileop_option)

    Rename a file, catching any errors and optionally warning/erroring.
- static void link_items (const StringArray &source_itemss, const bfs::path &dest_dir, bool overwrite)

    top-level link a list of source_paths (files, directories, symlinks), potentially including wildcards, from destination_dir, which must exist
- static void copy_items (const StringArray &source_items, const bfs::path &dest_dir, bool overwrite)

    copy a list of source_paths (files, directories, symlinks), potentially including wildcards into destination_dir, which must exist
- static void prepend_path_items (const StringArray &source_items)

    prepend any directories (including wildcards) found in source_items to the preferred environment path; this will update cached preferred path and PATH
- static bool check_equivalent_dest (const StringArray &source_items, const bfs::path &dest_dir)

    check whether any of the passed source items are filesystem equivalent to the destination path, return true if any one is equivalent to dest
- static bool find_driver (const StringArray &source_items, const bfs::path &search_driver)

    check whether the any of the passed source items (possibly including wildcards to be expanded) matches the passed search driver
- static bool link (const bfs::path &src_path, const bfs::path &dest_dir, bool overwrite)

    create link from dest_dir/src_path.filename() to a single path (file, dir, link) in source directory
- static bool recursive_copy (const bfs::path &src_path, const bfs::path &dest_dir, bool overwrite)

    Recrusive copy of src_path into dest_dir, with optional top-level overwrite (remove/recreate) of dest_dir/src_path.-filename()
- static bool prepend_path_item (const bfs::path &src_path, const bfs::path &dest_dir, bool overwrite)

    prepend the preferred env path with source path if it's a directory; this will update cached preferred path and manipulate PATH
- static bool check_equivalent (const bfs::path &src_path, const bfs::path &dest_dir, bool overwrite)

    return true if the src and dest are filesystem equivalent
- static bool find_file (const bfs::path &src_path, const bfs::path &search_file, bool overwrite)

    return true if the src_path is a regular file and has same filename as search_file
- static bool file_op_items (const file_op_function &file_op, const StringArray &source_paths, const bfs::path &dest_dir, bool overwrite)

    recursively perform file_op (copy, path adjust, etc.) on a list of source_paths (files, directories, symlinks), which potentially include wildcards, w.r.t. destination_dir
- static void set_preferred_path ()

    set/reset PATH to dakPreferredEnvPath
- static void set_preferred_path (const boost::filesystem::path &extra_path)

    set PATH to absolute(extra_path):dakPreferredEnvPath, without changing cached preferred PATH
- static void reset ()

    Resets the working directory "state" to its initial state when DAKOTA was launched.

Private Member Functions

- WorkdirHelper ()

    default constructor
- WorkdirHelper (const WorkdirHelper &)

    copy constructor
- ∼WorkdirHelper ()

    destructor
- WorkdirHelper & operator= (const WorkdirHelper &)

    assignment operator

Static Private Member Functions

- static bfs::path po_which (const std::string &driver_name)

  Returns the bfs::path for the analysis driver - POSIX-style implementation, returns empty if not found.
- static std::string init_startup_path ()

  Initializes class member, startupPATH.
- static std::string init_preferred_env_path ()

  Initializes class member, dakPreferredEnvPath.
- static std::vector< std::string > tokenize_env_path (const std::string &path)

  Tokenizes $PATH environment variable into a "list" of directories.

Static Private Attributes

- static std::string startupPWD = "."

  Value of $PWD var upon entry to dakota main()
- static std::string startupPATH = "."

  Value of $PATH (PATH% on windows) var upon entry to dakota main(), omitting any leading PATH= or Path=.
- static std::string dakPreferredEnvPath = "."

  Dakota preferred search PATH/Path = ".:startupPWD:startupPATH", omitting any leading PATH= or Path=.

14.302.1 Detailed Description

Utility class for cross-platform management of environment and paths. Including directory and file operations. On initialization, this class does not manipulate the present working directory, nor the PATH environment variable, but stores context to manipulate them later.

14.302.2 Member Function Documentation

14.302.2.1 void initialize ( ) [static]

initialize (at runtime) cached values for paths and environment

Initialize defers calls to Boost filesystem utilities until runtime (required on some operating systems.

References WorkdirHelper::dakPreferredEnvPath, WorkdirHelper::init_preferred_env_path(), WorkdirHelper::init_startup_path(), WorkdirHelper::startupPATH, and WorkdirHelper::startupPWD.

Referenced by Environment::Environment().

14.302.2.2 void prepend_preferred_env_path (const std::string & *extra_path*) [static]

Prepend cached preferredEnvPath with extra_path and update $PATH environment variable.

Overwrites $PATH with an additional directory prepended, typically for the purpose of ensuring templatedir is in the $PATH; updates cached preferred PATH and environment PATH, so exercise caution with repeated calls.

References WorkdirHelper::dakPreferredEnvPath, WorkdirHelper::set_environment(), and WorkdirHelper::startupPWD.

Referenced by WorkdirHelper::prepend_path_item().

14.302.2.3 bfs::path which (const std::string & *driver_name*) [static]

Returns the bfs::path for the analysis driver, supporting typical windows filename extensions, or empty if not found.

Uses string representing $PATH to locate an analysis driver on the host computer. Returns the path to the driver (as a string)

This version is a wrapper over the "plain ol' which" implementation, allowing an array of windows, 3-letter extensions to be checked.

References Dakota::get_pathext(), and WorkdirHelper::po_which().

Referenced by NIDRProblemDescDB::check_driver().

14.302.2.4 void split_wildcard (const std::string & *path_with_wc,* bfs::path & *search_dir,* bfs::path & *wild_card*) [static]

given a string with an optional path and a wildcard, e.g., /tmp/D∗.?pp, parse it into the search path /tmp (default .) and the wildcard D∗.?pp. Return wild_card as path to reduce wstring conversions

Input: path_with_wc; Output: search_dir, wild_card

Referenced by WorkdirHelper::file_op_items().

14.302.2.5 bfs::path concat_path (const bfs::path & *p_in,* const String & *tag*) [static]

concatenate a string onto the end of a path

NOTE: Could remove this function and use += at call sites, but seems convenient to keep (since path doesn't have operator+)

Referenced by ProcessApplicInterface::autotag_files(), ProcessApplicInterface::define_filenames(), ProcessApplicInterface::file_cleanup(), ProcessApplicInterface::get_workdir_name(), ProcessApplicInterface::read_results_files(), ProcessApplicInterface::remove_params_results_files(), and SysCallApplicInterface::system_call_file_test().

14.302.2.6 bool create_directory (const bfs::path & *dir_path,* short *mkdir_option*) [static]

Create a directory, with options for remove or error.

mkdir_option is DIR_CLEAN (remove and recreate), DIR_PERSIST (leave existing), or DIR_ERROR (don't allow existing) returns whether a new directory was created.

References Dakota::abort_handler(), and WorkdirHelper::recursive_remove().

Referenced by NonDMUQBayesCalibration::calibrate(), and ProcessApplicInterface::define_filenames().

14.302.2.7 void link_items (const StringArray & *source_items,* const bfs::path & *dest_dir,* bool *overwrite*) [static]

top-level link a list of source_paths (files, directories, symlinks), potentially including wildcards, from destination_dir, which must exist

Iterate source items (paths or wildcards), linking each of them from the destination. If overwrite, remove and replace any existing destination target, otherwise, allow to persist

References WorkdirHelper::file_op_items(), and WorkdirHelper::link().

Referenced by ProcessApplicInterface::define_filenames().

14.302.2.8 void copy_items (const StringArray & *source_items,* const bfs::path & *dest_dir,* bool *overwrite*) [static]

copy a list of source_paths (files, directories, symlinks), potentially including wildcards into destination_dir, which must exist

Iterate source items (paths or wildcards), copying each of them into the destination. If overwrite, remove and replace any existing destination target, otherwise, allow to persist

References WorkdirHelper::file_op_items(), and WorkdirHelper::recursive_copy().

Referenced by ProcessApplicInterface::define_filenames().

14.302.2.9 bool link (const bfs::path & *src_path,* const bfs::path & *dest_dir,* bool *overwrite*) [static]

create link from dest_dir/src_path.filename() to a single path (file, dir, link) in source directory

Assumes source file exists since it was iterated in the calling context. If overwrite, any existing file in dest_dir will be removed prior to creating the new link.

References Dakota::abort_handler().

Referenced by WorkdirHelper::link_items().

14.302.2.10 bool recursive_copy (const bfs::path & *src_path,* const bfs::path & *dest_dir,* bool *overwrite*) [static]

Recrusive copy of src_path into dest_dir, with optional top-level overwrite (remove/recreate) of dest_dir/src_path.-filename()

note dest_dir is the containing folder for the src_path contents to be placed in for consistency with other convenience functions (may need to reconsider)

References Dakota::abort_handler().

Referenced by WorkdirHelper::copy_items().

14.302.2.11 bool prepend_path_item (const bfs::path & *src_path,* const bfs::path & *dest_dir,* bool *overwrite*) [static]

prepend the preferred env path with source path if it's a directory; this will update cached preferred path and manipulate PATH

prepend the env path with source path if it's a directory or directory symlink

References Dakota::abort_handler(), and WorkdirHelper::prepend_preferred_env_path().

Referenced by WorkdirHelper::prepend_path_items().

14.302.2.12 bool file_op_items (const file_op_function & *file_op,* const StringArray & *source_items,* const bfs::path & *dest_dir,* bool *overwrite*) [static]

recursively perform file_op (copy, path adjust, etc.) on a list of source_paths (files, directories, symlinks), which potentially include wildcards, w.r.t. destination_dir

Iterator implementation for copy, link, etc file operation. Iterate source items (paths or wildcards), performing file_op on each w.r.t. destination. If overwrite, remove and replace any existing destination target (at top-level), otherwise, allow to persist. Return code true indicates abnormal behavior.

References WorkdirHelper::split_wildcard(), and Dakota::strcontains().

Referenced by WorkdirHelper::check_equivalent_dest(), WorkdirHelper::copy_items(), WorkdirHelper::find_driver(), WorkdirHelper::link_items(), and WorkdirHelper::prepend_path_items().

14.302.2.13 void set_preferred_path (const boost::filesystem::path & *extra_path*) [static]

set PATH to absolute(extra_path):dakPreferredEnvPath, without changing cached preferred PATH

If needed, convert the passed item to an absolute path (while could make sense to prepend a relative path, no current use cases) and prepend when setting environment. Does not update cached preferred path.

References WorkdirHelper::dakPreferredEnvPath, WorkdirHelper::rel_to_abs(), and WorkdirHelper::set_-environment().

14.302.2.14 bfs::path po_which (const std::string & *driver_name*) [static], [private]

Returns the bfs::path for the analysis driver - POSIX-style implementation, returns empty if not found.

For absolute driver_name, validates that is regular file. For relative, uses string representing $PATH (preferred path) to locate an analysis driver on the host computer. Returns the path to the driver, or empty if not found.

This is the "plain ol' which" impl that worked well, historically, on POSIX.

References Dakota::contains(), WorkdirHelper::dakPreferredEnvPath, and WorkdirHelper::tokenize_env_path().

Referenced by WorkdirHelper::which().

14.302.2.15 std::string init_startup_path ( ) [static], [private]

Initializes class member, startupPATH.

Gets the $PATH (PATH% on windows) and returns the std::string value

Referenced by WorkdirHelper::initialize().

14.302.2.16 std::string init_preferred_env_path ( ) [static], [private]

Initializes class member, dakPreferredEnvPath.

Prepends '.' and the startupPWD to the initial startup $PATH string so that analysis driver detection is more robust

References WorkdirHelper::startupPATH, and WorkdirHelper::startupPWD.

Referenced by WorkdirHelper::initialize().

14.302.2.17 std::vector< std::string > tokenize_env_path (const std::string & *env_path*) [static], [private]

Tokenizes $PATH environment variable into a "list" of directories.

Creates a a vector of directories (as an aid to search) by breaking up the $PATH environment variable (passed in as a string argument)

Referenced by WorkdirHelper::po_which().

The documentation for this class was generated from the following files:

- WorkdirHelper.hpp
- WorkdirHelper.cpp

Chapter 15

File Documentation

15.1 dakota_dll_api.cpp File Reference

This file contains a DakotaRunner class, which launches DAKOTA.

Namespaces

- Dakota

  The primary namespace for DAKOTA.

Functions

- void DAKOTA_DLL_FN dakota_create (int ∗dakota_ptr_int, const char ∗logname)

  create and configure a new DakotaRunner, adding it to list of instances
- int DAKOTA_DLL_FN dakota_readInput (int id, const char ∗dakotaInput)

  command DakotaRunner instance id to read from file dakotaInput
- void DAKOTA_DLL_FN dakota_get_variable_info (int id, char ∗∗∗pVarNames, int ∗pNumVarNames, char ∗∗∗pRespNames, int ∗pNumRespNames)

  return the variable and response names
- int DAKOTA_DLL_FN dakota_start (int id)

  command DakotaRunner instance id to start (plugin interface and run strategy)
- void DAKOTA_DLL_FN dakota_destroy (int id)

  delete Dakota runner instance id and remove from active list
- void DAKOTA_DLL_FN dakota_stop (int ∗id)

  command DakotaRunner instance id to stop execution
- const char ∗DAKOTA_DLL_FN dakota_getStatus (int id)

  return current results output as a string
- int get_mc_ptr_int ()

  get the DAKOTA pointer to ModelCenter
- void set_mc_ptr_int (int ptr_int)

  set the DAKOTA pointer to ModelCenter
- int get_dc_ptr_int ()

  get the DAKOTA pointer to ModelCenter current design point
- void set_dc_ptr_int (int ptr_int)

  set the DAKOTA pointer to ModelCenter current design point

15.1.1 Detailed Description

This file contains a DakotaRunner class, which launches DAKOTA.

15.1.2 Function Documentation

15.1.2.1 void DAKOTA_DLL_FN dakota_stop (int ∗ *id*)

command DakotaRunner instance id to stop execution

TODO: trick application to quit through the syscall interface or throw exception.

15.2 dakota_dll_api.h File Reference

API for DLL interactions.

Functions

- void DAKOTA_DLL_FN dakota_create (int ∗dakota_ptr_int, const char ∗logname)

  create and configure a new DakotaRunner, adding it to list of instances
- int DAKOTA_DLL_FN dakota_readInput (int id, const char ∗dakotaInput)

  command DakotaRunner instance id to read from file dakotaInput
- int DAKOTA_DLL_FN dakota_start (int id)

  command DakotaRunner instance id to start (plugin interface and run strategy)
- void DAKOTA_DLL_FN dakota_destroy (int id)

  delete Dakota runner instance id and remove from active list
- void DAKOTA_DLL_FN dakota_stop (int ∗id)

  command DakotaRunner instance id to stop execution
- const char ∗DAKOTA_DLL_FN dakota_getStatus (int id)

  return current results output as a string
- int DAKOTA_DLL_FN get_mc_ptr_int ()

  get the DAKOTA pointer to ModelCenter
- void DAKOTA_DLL_FN set_mc_ptr_int (int ptr_int)

  set the DAKOTA pointer to ModelCenter
- int DAKOTA_DLL_FN get_dc_ptr_int ()

  get the DAKOTA pointer to ModelCenter current design point
- void DAKOTA_DLL_FN set_dc_ptr_int (int ptr_int)

  set the DAKOTA pointer to ModelCenter current design point
- void DAKOTA_DLL_FN dakota_get_variable_info (int id, char ∗∗∗pVarNames, int ∗pNumVarNames, char ∗∗∗pRespNames, int ∗pNumRespNames)

  return the variable and response names

15.2.1 Detailed Description

API for DLL interactions.

15.2.2 Function Documentation

15.2.2.1 void DAKOTA_DLL_FN dakota_stop (int * *id*)

command DakotaRunner instance id to stop execution

TODO: trick application to quit through the syscall interface or throw exception.

15.3 dakota_linear_algebra.hpp File Reference

Dakota linear algebra utilities.

Namespaces

- Dakota

    The primary namespace for DAKOTA.

Functions

- void svd (RealMatrix &matrix, RealVector &singular_vals, RealMatrix &v_trans, bool compute_vectors=true)

    Compute the SVD of an arbitrary matrix A = USV^T.
- void singular_values (RealMatrix &matrix, RealVector &singular_values)

    compute the singular values without storing any singular vectors (A will be destroyed)
- int qr (RealMatrix &A)

    Compute an in-place QR factorization A = QR.
- int qr_rsolve (const RealMatrix &q_r, bool transpose, RealMatrix &rhs)

    *Perform a multiple right-hand sides Rinv * rhs solve using the R from a qr factorization.*
- double det_AtransA (RealMatrix &A)

    *Use SVD to compute det(A'*A), destroying A with the SVD.*

15.3.1 Detailed Description

Dakota linear algebra utilities. Convenience functions to perform Teuchos::LAPACK operations on Dakota Real-Matrix/RealVector

15.4 dakota_python.cpp File Reference

Namespaces

- Dakota

    The primary namespace for DAKOTA.

Functions

- void **print_version** ()
- std::vector< double > **get_variables_values** (const Dakota::LibraryEnvironment &env)
- py::array_t< double > **get_variables_values_numpy** (const Dakota::LibraryEnvironment &env)
- Real **get_response_fn_val** (const Dakota::LibraryEnvironment &env)
- Dakota::LibraryEnvironment * **create_libEnv** (const std::string &input_string)

- PYBIND11_MODULE (environment, m)

    Define a Python module that wraps a few top-level dakota functions Module name is really generic due to overly simple Python packaging scheme we're using.

15.4.1 Detailed Description

Python module wrapping top-level Dakota

15.5 dakota_tabular_io.hpp File Reference

Utility functions for reading and writing tabular data files Emerging utilities for tabular file I/O. For now, just extraction of capability from separate contexts to faciliate rework. These augment (and leverage) those in data_util.h.

Namespaces

- Dakota

    The primary namespace for DAKOTA.

Functions

- String **format_name** (unsigned short tabular_format)

    Translate tabular_format into a user-friendly name.
- void **print_expected_format** (std::ostream &s, unsigned short tabular_format, size_t num_rows, size_t num-_cols)

    Describe the expected data file format based on passed parameters.
- void **print_unexpected_data** (std::ostream &s, const String &filename, const String &context_message, unsigned short tabular_format)

    Print a warning if there's extra data in the file.
- void **open_file** (std::ifstream &data_file, const std::string &input_filename, const std::string &context_-message)

    open the file specified by name for reading, using passed input stream, presenting context-specific error on failure
- void **open_file** (std::ofstream &data_file, const std::string &output_filename, const std::string &context_-message)

    open the file specified by name for writing, using passed output stream, presenting context-specific error on failure
- void **close_file** (std::ifstream &data_file, const std::string &input_filename, const std::string &context_-message)

    close the file specified by name after reading, using passed input stream, presenting context-specific error on failure
- void **close_file** (std::ofstream &data_file, const std::string &output_filename, const std::string &context_-message)

    close the file specified by name after writing, using passed output stream, presenting context-specific error on failure
- void **write_header_tabular** (std::ostream &tabular_ostream, const std::string &eval_label, const std::string &iface_label, unsigned short tabular_format)

    Write the leading fields for the tabular header.
- void **write_header_tabular** (std::ostream &tabular_ostream, const std::string &eval_label, const StringArray &iface_labels, unsigned short tabular_format)

    Write the leading fields for the tabular header.
- void **write_header_tabular** (std::ostream &tabular_ostream, const Variables &vars, const Response &response, const std::string &eval_label, const std::string &interface_label, unsigned short tabular_format)

    Output the header row (labels) for a tabular data file for variables and responses, with variables in input spec order. Conditionally include interface ID. Primary uses: environment tabular data, pre-run output, surrogate approx evals.

- void **write_header_tabular** (std::ostream &tabular_ostream, const Variables &vars, const StringArray &addtnl_labels, const std::string &eval_label, const std::string &interface_label, unsigned short tabular_format)

    Output the header row (labels) for a tabular data file for variables and additional labels not tied to a response. Variables are in input spec order. Conditionally include interface ID. Primary uses: MCMC chain export, including calibration sigmas.

- void **append_header_tabular** (std::ostream &tabular_ostream, const Variables &vars, unsigned short tabular_format)

    append variable labels to the tabular header

- void **append_header_tabular** (std::ostream &tabular_ostream, const Variables &vars, size_t start_index, size_t num_items, unsigned short tabular_format)

    append range of variable labels to the tabular header

- void **append_header_tabular** (std::ostream &tabular_ostream, const StringArray &labels, unsigned short tabular_format)

    append an additional set of labels to the tabular header

- void **append_header_tabular** (std::ostream &tabular_ostream, const Response &response, unsigned short tabular_format, bool eol=true)

    append response labels to the tabular header

- void **write_leading_columns** (std::ostream &tabular_ostream, size_t eval_id)

    lower level helper for writing an evaluation id

- void **write_leading_columns** (std::ostream &tabular_ostream, const String &iface_id)

    lower level helper for writing an interface id

- void **write_leading_columns** (std::ostream &tabular_ostream, size_t eval_id, const String &iface_id, unsigned short tabular_format)

    Write the leading columns with an evaluation identifier and an interface identifier, as indicated by format bits.

- void **write_leading_columns** (std::ostream &tabular_ostream, size_t eval_id, const StringArray &iface_ids, unsigned short tabular_format)

    Write the leading columns with an evaluation identifier and one or more interface identifiers, as controlled by format bits.

- template<class T >
  void **write_scalar_tabular** (std::ostream &tabular_ostream, T val)

    Output a scalar as part of a row of tabular data.

- void **write_eol** (std::ostream &tabular_ostream)

    complete tabular row with EOL

- void **write_data_tabular** (std::ostream &tabular_ostream, const Variables &vars)

    Output a row of tabular data from a variables object. All active/inactive variables written in input spec order.

- void **write_data_tabular** (std::ostream &tabular_ostream, const Variables &vars, size_t start_index, size_t num_items)

    Output a row of tabular data from a variables object. All active/inactive variables written in input spec order.

- void **write_data_tabular** (std::ostream &tabular_ostream, const Response &response, bool eol=true)

    Output a row of tabular data from a response object.

- void **write_data_tabular** (std::ostream &tabular_ostream, const Response &response, size_t start_index, size_t num_items)

    Output a row of tabular data from a portion of a response object.

- void **write_data_tabular** (std::ostream &tabular_ostream, const Variables &vars, const String &iface, size_t counter, unsigned short tabular_format)

    Output a row of tabular data from a variables object. All active/inactive variables written in input spec order. Conditionally include interface ID. Primary uses: output of sampling sets.

- void **write_data_tabular** (std::ostream &tabular_ostream, const Variables &vars, const String &iface, const Response &response, size_t counter, unsigned short tabular_format)

    Output a row of tabular data from variables and response objects. All active/inactive variables written in input spec order. Conditionally include interface ID. Primary uses: environment tabular data, pre-run output, surrogate approx evals.

- void **write_data_tabular** (const std::string &output_filename, const std::string &context_message, const RealVectorArray &output_coeffs, const UShort2DArray &output_indices)

  PCE export: write freeform format file with whitespace-separated data where each row has num_fns reals from coeffs, followed by num_vars unsigned shorts from indices.
- bool **exists_extra_data** (std::istream &tabular_file)

  Check if an input stream contains unexpected additional data.
- StringArray **read_header_tabular** (std::istream &input_stream, unsigned short tabular_format)

  read and discard header line from the stream
- void **read_leading_columns** (std::istream &input_stream, unsigned short tabular_format)

  read leading columns [int eval_id [String iface_id]]
- void **read_leading_columns** (std::istream &input_stream, unsigned short tabular_format, int &eval_id, String &iface_id)

  read leading columns [int eval_id [String iface_id]]
- void **read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealVector &input_data, size_t num_entries, unsigned short tabular_format)

  read possibly header-annotated whitespace-separated data into a vector of length num_entries; if annotated then it's a column vector for now
- void **read_data_tabular** (const std::string &input_filename, const std::string &context_message, Variables vars, size_t num_fns, RealMatrix &vars_matrix, RealMatrix &resp_matrix, unsigned short tabular_format, bool verbose=false, bool use_var_labels=false, bool active_only=false)

  Tabular read for ApproximationInterface challenge data: read possibly header-annotated whitespace-separated data of possible mixed Variables, followed by num_fns, each into RealMatrix with minimal error checking.
- void **read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealVectorArray &input_coeffs, UShort2DArray &input_indices, unsigned short tabular_format, size_t num_vars, size_t num_fns)

  Tabular read for PCE import: read possibly header-annotated whitespace-separated data of unknown length where each row has num_fns reals followed by num_vars unsigned shorts; append data to arrays passed by reference.
- void **read_data_tabular** (const std::string &input_filename, const std::string &context_message, Variables vars, Response resp, PRPList &input_prp, unsigned short tabular_format, bool verbose=false, bool use_var_labels=false, bool active_only=false)

  Tabular read for DataFitSurrModel (build points): read whitespace-separated data with optional row and column headers into lists of Variables and Responses until out of data.
- void **read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealMatrix &input_matrix, size_t record_len, unsigned short tabular_format, bool verbose=false)

  Tabular read for import_approx_points_file: read whitespace-separated data with optional row and column headers into a single matrix, with length of record as specified and number of records to be determined by file content. The matrix is stored as record_len rows by num_records columns.
- void **read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealMatrix &input_matrix, size_t num_rows, size_t num_cols, unsigned short tabular_format, bool verbose=false)

  Tabular read for GPMSA data: read whitespace-separated data with optional row and column headers into a single matrix, with size as specified (one experiment per row)
- size_t **read_data_tabular** (const std::string &input_filename, const std::string &context_message, RealVectorArray &cva, IntVectorArray &diva, StringMulti2DArray &dsva, RealVectorArray &drva, unsigned short tabular_format, bool active_only, Variables vars)

  Tabular read for ParamStudy: read specified input data file into arrays with sizes specified by the passed vc_totals array.
- std::pair< size_t, bool > **read_data_tabular** (const std::string &input_filename, const std::string &context_message, size_t max_configs, VariablesArray &config_array, unsigned short tabular_format)

  Read up to max_configs configuration variables into config_array.

15.5.1 Detailed Description

Utility functions for reading and writing tabular data files Emerging utilities for tabular file I/O. For now, just extraction of capability from separate contexts to faciliate rework. These augment (and leverage) those in data_util.h.

Design/capability goals: Ability to read / write data with row/col headers or in free-form Detect premature end of file, report if extra data More consistent and reliable checks for file open errors Require right number of cols in header mode; only total data checking in free-form (likely) Allow comment character for header rows or even in data? variables vs. variables/responses for both read and write Should we support CSV? delimiter = ','; other? Verify treatment of trailing newline without reading a zero Allow reading into the transpose of the data structure

15.6 dll_tester.cpp File Reference

Test the DLL with a DAKOTA input file.

Functions

- int main (int argc, char ∗argv[])

    The main program for exercising the DLL API with a simple command-line.

15.6.1 Detailed Description

Test the DLL with a DAKOTA input file.

15.7 JEGAOptimizer.cpp File Reference

Contains the implementation of the JEGAOptimizer class.

Classes

- class JEGAOptimizer::Evaluator

    An evaluator specialization that knows how to interact with Dakota.
- class JEGAOptimizer::EvaluatorCreator

    A specialization of the JEGA::FrontEnd::EvaluatorCreator that creates a new instance of a Evaluator.
- class JEGAOptimizer::Driver

    A subclass of the JEGA front end driver that exposes the individual protected methods to execute the algorithm.

Namespaces

- Dakota

    The primary namespace for DAKOTA.

Functions

- template<typename T >
  string asstring (const T &val)

    Creates a string from the argument val using an ostringstream.

15.7.1 Detailed Description

Contains the implementation of the JEGAOptimizer class.

15.8 JEGAOptimizer.hpp File Reference

Contains the definition of the JEGAOptimizer class.

Classes

- class JEGAOptimizer

  A version of Dakota::Optimizer for instantiation of John Eddy's Genetic Algorithms (JEGA).
- class JEGATraits

  A version of TraitsBase specialized for John Eddy's Genetic Algorithms (JEGA).

Namespaces

- Dakota

  The primary namespace for DAKOTA.

15.8.1 Detailed Description

Contains the definition of the JEGAOptimizer class.

15.9 library_mode.cpp File Reference

file containing a mock simulator main for testing Dakota in library mode

Classes

- struct callback_data

Functions

- void fpinit_ASL ()
- void run_dakota_parse (const char ∗dakota_input_file)

  Run a Dakota LibraryEnvironment, mode 1: parsing an input file.
- void run_dakota_data ()

  Run a Dakota LibraryEnvironment, mode 2: from C++ API inserted data.
- void run_dakota_mixed (const char ∗dakota_input_file, bool mpirun_flag)

  Run a Dakota LibraryEnvironment, from string or input file input, supplemented with additional C++ API adjustments.
- void serial_interface_plugin (Dakota::LibraryEnvironment &env)

  Convenience function with simplest example of interface plugin: plugin a serial DirectApplicInterface that can be constructed independent of Dakota's configuration details.
- void parallel_interface_plugin (Dakota::LibraryEnvironment &env)

  Convenience function to plug a library client's interface into the appropriate model, demonstrating use of Dakota parallel configuration in constructing the plugin Interface on the right MPI_Comm.
- static void callback_function (Dakota::ProblemDescDB ∗db, void ∗ptr)

  Example: user-provided post-parse callback (Dakota::DbCallbackFunction)
- int main (int argc, char ∗argv[])

  A mock simulator main for testing Dakota in library mode.

Variables

- static const char serial_input [ ]

  Default Dakota input string for serial case (rosenbrock):
- static const char parallel_input [ ]

  Default Dakota input string for parallel case (text_book)

15.9.1 Detailed Description

file containing a mock simulator main for testing Dakota in library mode

15.9.2 Function Documentation

15.9.2.1 void fpinit_ASL ( )

Floating-point initialization from AMPL: switch to 53-bit rounding if appropriate, to eliminate some cross-platform differences.

Referenced by main().

15.9.2.2 void run_dakota_parse (const char * *dakota_input_file*)

Run a Dakota LibraryEnvironment, mode 1: parsing an input file.

Simplest library case: this function parses from an input file to define the ProblemDescDB data.

References Environment::execute(), ProgramOptions::input_file(), Environment::mpi_manager(), MPIManager::mpirun_flag(), parallel_interface_plugin(), serial_interface_plugin(), and MPIManager::world_rank().

Referenced by main().

15.9.2.3 void run_dakota_data ( )

Run a Dakota LibraryEnvironment, mode 2: from C++ API inserted data.

Rather than parsing from an input file, this function populates Data class objects directly using a minimal specification and relies on constructor defaults and post-processing in post_process() to fill in the rest.

References DataInterface::data_rep(), DataResponses::data_rep(), DataVariables::data_rep(), DataMethod::data_rep(), LibraryEnvironment::done_modifying_db(), Environment::execute(), Environment::exit_mode(), DataResponsesRep::gradientType, DataResponsesRep::hessianType, LibraryEnvironment::insert_nodes(), DataMethodRep::methodName, Environment::mpi_manager(), MPIManager::mpirun_flag(), ParallelLibrary::mpirun_flag(), DataVariablesRep::numContinuousDesVars, DataResponsesRep::numNonlinearIneqConstraints, DataResponsesRep::numObjectiveFunctions, parallel_interface_plugin(), Environment::parallel_library(), serial_interface_plugin(), and ParallelLibrary::world_rank().

Referenced by main().

15.9.2.4 void run_dakota_mixed (const char * *dakota_input_file,* bool *mpirun_flag*)

Run a Dakota LibraryEnvironment, from string or input file input, supplemented with additional C++ API adjustments.

Function to encapsulate the Dakota object instantiations for mode 3: mixed parsing and direct updating.

This function showcases multiple features. For parsing, either an input file (dakota_input_file != NULL) or a default input string (dakota_input_file == NULL) are shown. This parsed input is then mixed with input from three sources: (1) input from a user-supplied callback function, (2) updates to the DB prior to Environment instantiation, (3) updates directly to Iterators/Models following Environment instantiation.

References callback_function(), LibraryEnvironment::done_modifying_db(), ProgramOptions::echo_input(), Environment::execute(), LibraryEnvironment::filtered_model_list(), ProblemDescDB::get_sa(), ProgramOptions::input_file(), ProgramOptions::input_string(), Environment::mpi_manager(), MPIManager::mpirun_flag(), parallel_input, parallel_interface_plugin(), Environment::parallel_library(), Environment::problem_description_db(), ProblemDescDB::resolve_top_method(), callback_data::rosen_cdv_upper_bd, serial_input, serial_interface_plugin(), ProblemDescDB::set(), and ParallelLibrary::world_rank().

Referenced by main().

15.9.2.5 void serial_interface_plugin (Dakota::LibraryEnvironment & *env*)

Convenience function with simplest example of interface plugin: plugin a serial DirectApplicInterface that can be constructed independent of Dakota's configuration details.

Demonstration of simple plugin where client code doesn't require access to detailed Dakota data (such as Model-based parallel configuration information) to construct the DirectApplicInterface. This example plugs-in a derived serial direct application interface instance ("plugin_rosenbrock").

References Dakota::abort_handler(), LibraryEnvironment::plugin_interface(), and Environment::problem_description_db().

Referenced by run_dakota_data(), run_dakota_mixed(), and run_dakota_parse().

15.9.2.6 void parallel_interface_plugin (Dakota::LibraryEnvironment & *env*)

Convenience function to plug a library client's interface into the appropriate model, demonstrating use of Dakota parallel configuration in constructing the plugin Interface on the right MPI_Comm.

From a filtered list of Model candidates, plug-in a derived direct application interface instance ("plugin_text_book" for parallel). This approach provides more complete access to the Model, e.g., for access to analysis communicators.

References Dakota::abort_handler(), Interface::assign_rep(), LibraryEnvironment::filtered_model_list(), ProblemDescDB::get_db_model_node(), Environment::problem_description_db(), and ProblemDescDB::set_db_model_nodes().

Referenced by run_dakota_data(), run_dakota_mixed(), and run_dakota_parse().

15.9.2.7 static void callback_function (Dakota::ProblemDescDB ∗ *db*, void ∗ *ptr*) [static]

Example: user-provided post-parse callback (Dakota::DbCallbackFunction)

Example of user-provided callback function (an instance of Dakota::DbCallbackFunction) to override input provided by parsed Dakota input file or input string data.

References Dakota::contains(), ProblemDescDB::get_sa(), ProblemDescDB::get_ushort(), ProblemDescDB::resolve_top_method(), callback_data::rosen_cdv_upper_bd, and ProblemDescDB::set().

Referenced by run_dakota_mixed().

15.9.2.8 int main (int *argc*, char ∗ *argv[ ]*)

A mock simulator main for testing Dakota in library mode.

Overall Usage: dakota_library_mode [-mixed] [dakota.in]

Uses alternative instantiation syntax as described in the library mode documentation within the Developers Manual. Tests several problem specification modes:

(1) run_dakota_parse: reads all problem specification data from a Dakota input file. Usage: dakota_library_mode dakota.in

(2) run_dakota_data: creates all problem specification from direct Data instance instantiations in the C++ code. Usage: dakota_library_mode

(3) run_dakota_mixed: a mixture of input parsing and direct data updates, where the data updates occur: (a) via the DB during Environment instantiation, and (b) via Iterators/Models following Environment instantiation. Usage: dakota_library_mode -mixed (input from default string) dakota_library_mode -mixed dakota.in (input from specified file)

Serial cases use a plugin rosenbrock model, while parallel cases use textbook.

References MPIManager::detect_parallel_launch(), fpinit_ASL(), Dakota::mpi_debug_hold(), run_dakota_data(), run_dakota_mixed(), and run_dakota_parse().

15.9.3 Variable Documentation

15.9.3.1 const char serial_input[ ] [static]

Initial value:

```
=
  "     method,"
  "             optpp_q_newton"
  "               max_iterations = 50"
  "               convergence_tolerance = 1e-4"
  "     variables,"
  "             continuous_design = 2"
  "               descriptors 'x1' 'x2'"
  "     interface,"
  "             direct"
  "               analysis_driver = 'plugin_rosenbrock'"
  "     responses,"
  "             num_objective_functions = 1"
  "             analytic_gradients"
  "             no_hessians"
```

Default Dakota input string for serial case (rosenbrock):

Referenced by run_dakota_mixed().

15.9.3.2 const char parallel_input[ ] [static]

Initial value:

```
=
  "     method,"
  "             optpp_q_newton"
  "               max_iterations = 50"
  "               convergence_tolerance = 1e-4"
  "     variables,"
  "             continuous_design = 2"
  "               descriptors 'x1' 'x2'"
  "     interface,"
  "             direct"
  "               analysis_driver = 'plugin_text_book'"
  "     responses,"
  "             num_objective_functions = 1"
  "             num_nonlinear_inequality_constraints = 2"
  "             analytic_gradients"
  "             no_hessians"
```

Default Dakota input string for parallel case (text_book)

Referenced by run_dakota_mixed().

15.10 library_split.cpp File Reference

file containing a mock simulator main for testing DAKOTA in library mode on a split communicator

Functions

- void manage_mpi (MPI_Comm &my_comm, int &color)

  Split MPI_COMM_WORLD, returning the comm and color.
- void gen_dakota_input (const int &color, std::string &input)

  Return the appropriate DAKOTA input based on color (1 or 2)
- void run_dakota (const MPI_Comm &comm, const std::string &input, const int &color)

  Launch DAKOTA on passed communicator, tagging output/error with color.
- void collect_results ()

  Wait for and collect results from DAKOTA runs.
- int main (int argc, char ∗argv[])

  Driver routine for testing library mode with partitioned MPI_Comm. This test fixture requires MPI and can be run on 3–8 processors.

15.10.1 Detailed Description

file containing a mock simulator main for testing DAKOTA in library mode on a split communicator

15.11 main.cpp File Reference

file containing the main program for DAKOTA

Functions

- void fpinit_ASL ()
- int main (int argc, char ∗argv[])

  The main DAKOTA program.

15.11.1 Detailed Description

file containing the main program for DAKOTA

15.11.2 Function Documentation

15.11.2.1 void fpinit_ASL ( )

Floating-point initialization from AMPL: switch to 53-bit rounding if appropriate, to eliminate some cross-platform differences.

15.11.2.2 int main (int *argc*, char ∗ *argv[]*)

The main DAKOTA program.

Manage command line inputs, input files, restart file(s), output streams, and top level parallel iterator communicators. Instantiate the ExecutableEnvironment and invoke its execute() virtual function.

References Environment::check(), ExecutableEnvironment::execute(), fpinit_ASL(), Dakota::mpi_debug_hold(), and Dakota::register_signal_handlers().

15.12 QUESOImpl.hpp File Reference

Classes

- class QuesoJointPdf< V, M >

    Dakota specialization of QUESO generic joint PDF.
- class QuesoVectorRV< V, M >

    Dakota specialization of QUESO vector-valued random variable.
- class DerivInformedPropCovTK< V, M >

    Dakota transition kernel that updates proposal covariance based on derivatives (for random walk case)
- class DerivInformedPropCovLogitTK< V, M >

    Dakota transition kernel that updates proposal covariance based on derivatives (for logit random walk case)
- class TKFactoryDIPC

    Custom RW TKfactory: passes Dakota QUESO instance pointer to the TK at build.
- class TKFactoryDIPCLogit

    Custom Logit RW TKfactory: passed Dakota QUESO instance pointer to the TK at build.

Namespaces

- Dakota

    The primary namespace for DAKOTA.

15.12.1 Detailed Description

QUESO specializations for evaluations and utilities

15.13 restart_util.cpp File Reference

file containing the DAKOTA restart utility main program

Namespaces

- Dakota

    The primary namespace for DAKOTA.

Functions

- void print_usage (std::ostream &s)

    print restart utility help message
- void print_restart (StringArray pos_args, String print_dest)

    print a restart file
- void print_restart_pdb (StringArray pos_args, String print_dest)

    print a restart file (PDB format)
- void print_restart_tabular (StringArray pos_args, String print_dest, unsigned short tabular_format, int tabular_precision)

    print a restart file (tabular format)
- void read_neutral (StringArray pos_args)

    read a restart file (neutral file format)
- void repair_restart (StringArray pos_args, String identifier_type)

repair a restart file by removing corrupted evaluations
- void concatenate_restart (StringArray pos_args)

  concatenate multiple restart files
- int main (int argc, char ∗argv[])

  The main program for the DAKOTA restart utility.

15.13.1 Detailed Description

file containing the DAKOTA restart utility main program

15.13.2 Function Documentation

15.13.2.1 int main (int *argc*, char ∗ *argv[]*)

The main program for the DAKOTA restart utility.

Parse command line inputs and invoke the appropriate utility function (print_restart(), print_restart_tabular(), read_-neutral(), repair_restart(), or concatenate_restart()).

References Dakota::concatenate_restart(), Dakota::print_restart(), Dakota::print_restart_pdb(), Dakota::print_-restart_tabular(), Dakota::print_usage(), Dakota::read_neutral(), Dakota::repair_restart(), and Dakota::write_-precision.

15.14 surrogates_python.cpp File Reference

Classes

- class PyPolyReg

  Extend PolynomialRegression with a new type for Python.

Functions

- ParameterList convert_options (pybind11::dict pydict)

  Convert Python dictionary to options list.
- PYBIND11_MODULE (surrogates, m)

  Define a Python module that wraps a few surrogates classes Module name is really generic due to overly simple Python packaging scheme we're using.

15.14.1 Detailed Description

Python module wrapping surrogates modules

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