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DAKOTA, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis

Version 3.0 Developers Manual

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Abstract

The DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) 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, analytic reliability, and stochastic finite element methods; parameter estimation with nonlinear least squares methods; and sensitivity 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 serves as a developers manual for the DAKOTA software and describes the DAKOTA class hierarchies and their interrelationships. It derives directly from annotation of the actual 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 (Design Analysis Kit for Optimization and Terascale Applications) toolkit provides a flexible, extensible interface between analysis codes and iteration methods. DAKOTA contains algorithms for optimization with gradient and nongradient-based methods, uncertainty quantification with sampling, analytic reliability, and stochastic finite element methods, parameter estimation with nonlinear least squares methods, and sensitivity/primary effects analysis with design of experiments and parameter study capabilities. These capabilities may be used on their own or as components within advanced strategies for 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 as well as a platform for rapid prototyping of advanced solution methodologies.

The Developers Manual focuses on documentation of the class structures used by the DAKOTA system. It derives directly from annotation of the actual source code. For information on input command syntax, refer to the `Reference Manual`, and for a tour of DAKOTA features and capabilities, refer to the Users Manual.

1.2 Overview of DAKOTA

In the DAKOTA system, the *strategy* creates and manages *iterators* and *models*. In the simplest case, the strategy creates a single iterator and a single model and executes the iterator on the model to perform a single study. In a more advanced case, a hybrid optimization strategy might manage a global optimizer operating on a low-fidelity model in coordination with a local optimizer operating on a high-fidelity model. And on the high end, a surrogate-based optimization under uncertainty strategy would employ an uncertainty quantification iterator nested within an optimization iterator and would employ truth models layered

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 broad array of specializations for supporting a variety of studies. In a DAKOTA input file, the user specifies these components through strategy, method, variables, interface, and responses keyword specifications.

The extensive use of class hierarchies provides a clear direction 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 small number 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 software components are presented in the following sections using a top-down order.

1.2.1 Strategies

Class hierarchy: DakotaStrategy.

Strategies provide a control layer for creation and management of iterators and models. Specific strategies include:

- SingleMethodStrategy: the simplest strategy. A single iterator is run on a single model to perform a single study.
- MultilevelOptStrategy: hybrid optimization using a succession of iterators employing a succession of models of varying fidelity. The best results obtained are passed from one iterator to the next.
- SurrBasedOptStrategy: surrogate-based optimization. Employs a single iterator with a LayeredModel (either data fit or hierarchical). A sequence of approximate optimizations is performed, each of which involves build, optimize, and verify steps.
- NonDOptStrategy: optimization under uncertainty (OUU). Employs a single iterator with a NestedModel. In OUU approaches involving surrogates, NestedModels and LayeredModels can be chained together in a variety of ways using recursion in sub-models.
- BranchBndStrategy: mixed integer nonlinear programming using the PICO library for parallel branch and bound. Employs a single iterator with a single model, but runs multiple instances of the iterator concurrently for different variable bounds within the model.
- ConcurrentStrategy: two similar algorithms are available: (1) multi-start iteration from several different starting points, and (2) pareto set optimization for several different multiobjective weightings. Employs a single iterator with a single model, but runs multiple instances of the iterator concurrently for different settings within the model.

1.2.2 Iterators

Class hierarchy: DakotaIterator.

The iterator hierarchy contains a variety of iterative algorithms for optimization, uncertainty quantification, nonlinear least squares, design of experiments, and parameter studies.

- Optimization: DakotaOptimizer inherits from DakotaIterator and provides a base class for DOTOptimizer, CONMINOptimizer, NPSOLOptimizer, SNLLOptimizer, and SGOPTOptimizer.

- Uncertainty quantification: DakotaNonD inherits from DakotaIterator and provides a base class for NonDProbability, NonDAdvMeanValue, and NonDPCE.
- Parameter estimation: a Gauss-Newton least squares solver is provided as part of SNLLOptimizer.
- Design of experiments: DACEIterator inherits directly from DakotaIterator. NonDProbability from the uncertainty quantification branch can also be used for this purpose.
- Parameter studies: ParamStudy inherits directly from DakotaIterator.

1.2.3 Models

Class hierarchy: DakotaModel.

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.

- SingleModel: variables are mapped into responses using a single DakotaInterface object. No sub-iterators or sub-models are used.
- LayeredModel: 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). LayeredModel has two derived classes: SurrLayeredModel for data fit surrogates and HierLayeredModel 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 in the response evaluation for the top level model, but rather used in separate build and correction steps.
- NestedModel: variables are mapped into responses using a combination of an optional DakotaInterface and a sub-iterator/sub-model pair. The relationship of the sub-iterators and sub-models is considered to be ”nested” since they are executed on every evaluation of the top level model as part of the response computation.

1.2.4 Variables

Class hierarchy: DakotaVariables.

The DakotaVariables class hierarchy manages design, uncertain, and state variable types for continuous and discrete domain types. This hierarchy is specialized according to various views of the data.

- FundamentalVariables: variable and domain type distinctions are retained, i.e. separate arrays for design, uncertain, and state variables types and for continuous and discrete domains.
- AllVariables: variable types are combined and domain type distinction is retained, i.e. design, uncertain, and state variable types combined into a single continuous variables array and a single discrete variables array.
- MergedVariables: variable type distinction is retained and domain types are combined, i.e. continuous and discrete variables merged into continuous arrays for design, uncertain, and state variable types.
- AllMergedVariables: variable and domain types are combined, i.e. design, uncertain, and state variable types combined (all) and continuous and discrete domain types combined (merged). The result is a single array of continuous variables.

The DakotaVarConstraints hierarchy contains the same specializations for managing linear and bound constraints on the variables (see FundamentalVarConstraints, AllVarConstraints, MergedVarConstraints, AllMergedVarConstraints).

1.2.5 Interfaces

Class hierarchy: DakotaInterface.

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

- SysCallApplicInterface: the simulation is invoked using a system call (the C function system()). Asynchronous invocation utilizes a background system call. Utilizes the SysCallAnalysisCode class to define syntax for input filter, analysis code, output filter, or combined spawning, which in turn utilize the CommandShell overloaded operator definitions.
- ForkApplicInterface: the simulation is invoked using a fork (the fork/exec/wait family of functions). Asynchronous invocation utilizes a nonblocking fork. Utilizes the ForkAnalysisCode class for lower level fork operations.
- XMLApplicInterface: the simulation is invoked using an XML packet passed across a socket communication. This capability is experimental and still under development.

and the following semi-intrusive approach

- DirectFnApplicInterface: the simulation is linked into the DAKOTA executable and is invoked using a procedure call. Asynchronous invocation utilizes a nonblocking thread (capability not yet available).

are supported. 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 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 DakotaApproximation objects, one per response function, which allows mixing of approximation types (using the DakotaApproximation derived classes: ANNSurf, KrigingSurf, MARSSurf, RespSurf, HermiteSurf, and TaylorSurf).

1.2.6 Responses

Class: DakotaResponse.

Responses provide an abstract data representation of response functions, their gradients, and their Hessians which can be interpreted as an objective function and constraints (optimization data set), residual functions

(least squares data set), or generic response functions (uncertainty and parameter study data sets). This class is not currently part of a class hierarchy, since the abstraction has been sufficiently general and has not required specialization.

1.3 Related Components

A variety of services are provided in DAKOTA for parallel computing, failure capturing, restart, graphics, etc. In addition, the execution of function evaluations is a core component of DAKOTA involving several class hierarchies. An overview of the classes and member functions involved in performing function evaluations is included below.

1.3.1 Services

- Multilevel parallel computing: DAKOTA supports up to 4 nested levels of parallelism: a strategy can manage concurrent iterators, each of which manages concurrent function evaluations, each of which contains 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 ConcurrentStrategy, ApplicationInterface, and ForkApplicInterface.
- Parsing: DAKOTA employs the Input Deck Reader (IDR) parser to retrieve information from user input files. Parsing options are processed in CommandLineHandler and parsing occurs in main.C. IDR populates data within the ProblemDescDB support class, which maintains the strategy specification and lists of DataMethod, DataVariables, DataInterface, and DataResponses specifications. Instructions 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 processed in CommandLineHandler, restart file management occurs in main.C, and restart file insertions occur in ApplicationInterface. The dakota_restart_util executable, built from restart_util.C, 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: DakotaStrategy, DakotaIterator, DakotaModel, DakotaVariables, DakotaVarConstraints, DakotaInterface, and DakotaApproximation. The latter idiom provides for memory efficiency in heavily used classes which do not involve a class hierarchy. Currently, only the DakotaResponse class uses this idiom.
- Graphics: DAKOTA provides 2D graphics using Motif widgets and 3D graphics from the PLPLOT package. Graphics data can also be catalogued in a tabular data file for post-processing with 3rd party tools such as Matlab, Tecplot, etc. All of these capabilities are encapsulated within the DakotaGraphics class.

1.3.2 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.

For a synchronous (i.e., blocking) mapping of parameters to responses, an iterator invokes DakotaModel::compute_response() 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:

- DakotaModel::compute_response() utilizes DakotaModel::derived_compute_response() for portions of the response computation specific to derived model classes.
- DakotaModel::derived_compute_response() directly or indirectly invokes DakotaInterface::map().
- DakotaInterface::map() utilizes ApplicationInterface::derived_map() for portions of the mapping specific to derived application interface classes.

For an asynchronous (i.e., nonblocking) mapping of parameters to responses, an iterator invokes DakotaModel::asynch_compute_response() multiple times to queue asynchronous jobs and then invokes either DakotaModel::synchronize() or DakotaModel::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:

- DakotaModel::asynch_compute_response() utilizes DakotaModel::derived_asynch_compute_response() for portions of the response computation specific to derived model classes.
- This derived model class function directly or indirectly invokes DakotaInterface::map() in asynchronous mode, which adds the job to a scheduling queue.
- DakotaModel::synchronize() or DakotaModel::synchronize_nowait() utilize DakotaModel::derived_synchronize() or DakotaModel::derived_synchronize_nowait() for portions of the scheduling process specific to derived model classes.
- These derived model class functions directly or indirectly invoke DakotaInterface::synch() or DakotaInterface::synch_nowait().
- For application interfaces, these interface synchronization functions are responsible for performing evaluation scheduling in one of the following modes:
  - asynchronous local mode (using ApplicationInterface::asynchronous_local_evaluations() or ApplicationInterface::asynchronous_local_evaluations_nowait())
  - message passing mode (using ApplicationInterface::self_schedule_evaluations() or ApplicationInterface::static_schedule_evaluations() on the iterator master and ApplicationInterface::serve_evaluations_synch() or ApplicationInterface::serve_evaluations_peer() on the servers)
  - hybrid mode (using ApplicationInterface::self_schedule_evaluations() or ApplicationInterface::static_schedule_evaluations() on the iterator master and ApplicationInterface::serve_evaluations_asynch() on the servers)
- These scheduling functions utilize ApplicationInterface::derived_map() and ApplicationInterface::derived_map_asynch() for portions of asynchronous job launching specific to derived application interface classes, as well as ApplicationInterface::derived_synch() and ApplicationInterface::derived_synch_nowait() for portions of job capturing specific to derived application interface classes.

This 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 (ForkApplicInterface::synchronous_local_analyses(), ForkApplicInterface::asynchronous_local_analyses(), ApplicationInterface::self_schedule_analyses(), ApplicationInterface::serve_analyses_synch(), ForkApplicInterface::serve_analyses_asynch()) 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.

1.4 Additional Resources

Additional development resources include:

- Recommended Practices for DAKOTA Development
- Instructions for Modifying DAKOTA's Input Specification
- Project web pages are maintained at `http://endo.sandia.gov/DAKOTA` with software specifics and documentation pointers provided at `http://endo.sandia.gov/DAKOTA/software.html`, and a list of publications provided at `http://endo.sandia.gov/DAKOTA/references.html`

Chapter 2

DAKOTA Hierarchical Index

2.1 DAKOTA Class Hierarchy

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

Chapter 3

DAKOTA Compound Index

3.1 DAKOTA Compound List

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

Chapter 4

DAKOTA File Index

4.1 DAKOTA File List

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

Chapter 5

DAKOTA Page Index

5.1 DAKOTA Related Pages

Here is a list of all related documentation pages:

Chapter 6

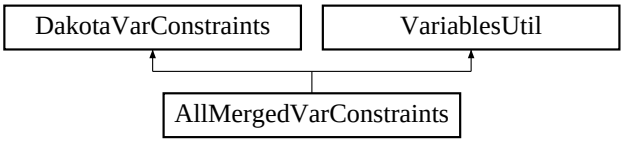
DAKOTA Class Documentation

6.1 AllMergedVarConstraints Class Reference

Derived class within the DakotaVarConstraints hierarchy which combines the all and merged data views.

`#include <AllMergedVarConstraints.H>`

Inheritance diagram for AllMergedVarConstraints::



Public Methods

- AllMergedVarConstraints (const ProblemDescDB &problem_db)
  constructor.
- ~AllMergedVarConstraints ()
  destructor.
- const DakotaRealVector & continuous_lower_bounds () const
  return the active continuous variable lower bounds.
- void continuous_lower_bounds (const DakotaRealVector &c_l_bnds)
  set the active continuous variable lower bounds.
- const DakotaRealVector & continuous_upper_bounds () const
  return the active continuous variable upper bounds.
- void continuous_upper_bounds (const DakotaRealVector &c_u_bnds)

set the active continuous variable upper bounds.

- const DakotaIntVector & discrete_lower_bounds () const

  return the active discrete variable lower bounds.

- void discrete_lower_bounds (const DakotaIntVector &d_l_bnds)

  set the active discrete variable lower bounds.

- const DakotaIntVector & discrete_upper_bounds () const

  return the active discrete variable upper bounds.

- void discrete_upper_bounds (const DakotaIntVector &d_u_bnds)

  set the active discrete variable upper bounds.

- void write (ostream &s) const

  write a variable constraints object to an ostream.

- void read (istream &s)

  read a variable constraints object from an istream.

Private Attributes

- DakotaRealVector allMergedLowerBnds

  a continuous lower bounds array combining design, uncertain, and state variable types and merging continuous and discrete domains. The order is continuous design, discrete design, uncertain, continuous state, and discrete state.

- DakotaRealVector allMergedUpperBnds

  a continuous upper bounds array combining design, uncertain, and state variable types and merging continuous and discrete domains. The order is continuous design, discrete design, uncertain, continuous state, and discrete state.

- DakotaIntVector emptyIntVector

  an empty int vector returned in get functions when there are no variables corresponding to the request.

6.1.1 Detailed Description

Derived class within the DakotaVarConstraints hierarchy which combines the all and merged data views.

Derived variable constraints classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The AllMergedVarConstraints derived class combines design, uncertain, and state variable types (all) and continuous and discrete domain types (merged). The result is a single continuous lower bounds array (allMergedLowerBnds) and a single continuous upper bounds array (allMergedUpperBnds). No iterators/strategies currently use this approach; it is included for completeness and future capability.

6.1.2 Constructor & Destructor Documentation

6.1.2.1 AllMergedVarConstraints::AllMergedVarConstraints (const ProblemDescDB & *problem_db*)

constructor.

Extract fundamental variable bounds and combine them into allMergedLowerBnds and allMergedUpperBnds using utilities from VariablesUtil.

The documentation for this class was generated from the following files:

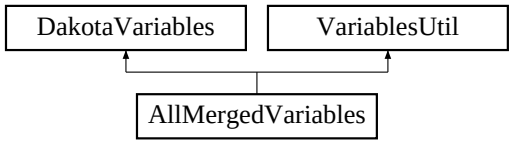
- AllMergedVarConstraints.H
- AllMergedVarConstraints.C

6.2 AllMergedVariables Class Reference

Derived class within the DakotaVariables hierarchy which combines the all and merged data views.

`#include <AllMergedVariables.H>`

Inheritance diagram for AllMergedVariables::



Public Methods

- AllMergedVariables ()
  default constructor.
- AllMergedVariables (const ProblemDescDB &problem_db)
  standard constructor.
- ~AllMergedVariables ()
  destructor.
- size_t tv () const
  Returns total number of vars.
- size_t cv () const
  Returns number of active continuous vars.
- size_t dv () const
  Returns number of active discrete vars.
- const DakotaRealVector & continuous_variables () const
  return the active continuous variables.
- void continuous_variables (const DakotaRealVector &c_vars)
  set the active continuous variables.
- const DakotaIntVector & discrete_variables () const
  return the active discrete variables.
- void discrete_variables (const DakotaIntVector &d_vars)
  set the active discrete variables.
- const DakotaStringArray & continuous_variable_labels () const

return the active continuous variable labels.

- void continuous_variable_labels (const DakotaStringArray &cv_labels)
  set the active continuous variable labels.
- const DakotaStringArray & discrete_variable_labels () const
  return the active discrete variable labels.
- void discrete_variable_labels (const DakotaStringArray &dv_labels)
  set the active discrete variable labels.
- const DakotaRealVector & inactive_continuous_variables () const
  return the inactive continuous variables.
- void inactive_continuous_variables (const DakotaRealVector &i_c_vars)
  set the inactive continuous variables.
- const DakotaIntVector & inactive_discrete_variables () const
  return the inactive discrete variables.
- void inactive_discrete_variables (const DakotaIntVector &i_d_vars)
  set the inactive discrete variables.
- size_t acv () const
  returns total number of continuous vars.
- size_t adv () const
  returns total number of discrete vars.
- DakotaRealVector all_continuous_variables () const
  returns a single array with all continuous variables.
- DakotaIntVector all_discrete_variables () const
  returns a single array with all discrete variables.
- void read (istream &s)
  read a variables object from an istream.
- void write (ostream &s) const
  write a variables object to an ostream.
- void read_annotated (istream &s)
  read a variables object in annotated format from an istream.
- void write_annotated (ostream &s) const
  write a variables object in annotated format to an ostream.
- void read (DakotaBiStream &s)
  read a variables object from the binary restart stream.

- void write (DakotaBoStream &s) const

  write a variables object to the binary restart stream.

- void read (UnPackBuffer &s)

  read a variables object from a packed MPI buffer.

- void write (PackBuffer &s) const

  write a variables object to a packed MPI buffer.

Private Methods

- void copy_rep (const DakotaVariables *vars_rep)

  Used by copy() to copy the contents of a letter class.

Private Attributes

- DakotaRealVector allMergedVars

  a continuous array combining design, uncertain, and state variable types and merging continuous and discrete domains. The order is continuous design, discrete design, uncertain, continuous state, and discrete state.

- DakotaStringArray allMergedLabels

  an array containing labels for continuous design, discrete design, uncertain, continuous state, and discrete state variables.

- DakotaRealVector emptyRealVector

  an empty real vector returned in get functions when there are no variables corresponding to the request.

- DakotaIntVector emptyIntVector

  an empty int vector returned in get functions when there are no variables corresponding to the request.

- DakotaStringArray emptyStringArray

  an empty label array returned in get functions when there are no variables corresponding to the request.

Friends

- int operator== (const AllMergedVariables &vars1, const AllMergedVariables &vars2)

  equality operator.

6.2.1 Detailed Description

Derived class within the DakotaVariables hierarchy which combines the all and merged data views.

Derived variables classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The AllMergedVariables derived class combines design, uncertain,

and state variable types (all) and continuous and discrete domain types (merged). The result is a single array of continuous variables (allMergedVars). No iterators/strategies currently use this approach; it is included for completeness and future capability.

6.2.2 Constructor & Destructor Documentation

6.2.2.1 AllMergedVariables::AllMergedVariables (const ProblemDescDB & *problem_db*)

standard constructor.

Extract fundamental variable types and labels and combine them into allMergedVars and allMergedLabels using utilities from VariablesUtil.

The documentation for this class was generated from the following files:

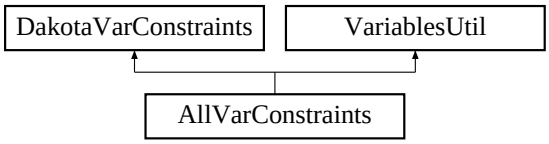
- AllMergedVariables.H
- AllMergedVariables.C

6.3 AllVarConstraints Class Reference

Derived class within the DakotaVarConstraints hierarchy which employs the all data view.

`#include <AllVarConstraints.H>`

Inheritance diagram for AllVarConstraints::



Public Methods

- AllVarConstraints (const ProblemDescDB &problem_db)
  constructor.
- ~AllVarConstraints ()
  destructor.
- const DakotaRealVector & continuous_lower_bounds () const
  return the active continuous variable lower bounds.
- void continuous_lower_bounds (const DakotaRealVector &c_l_bnds)
  set the active continuous variable lower bounds.
- const DakotaRealVector & continuous_upper_bounds () const
  return the active continuous variable upper bounds.
- void continuous_upper_bounds (const DakotaRealVector &c_u_bnds)
  set the active continuous variable upper bounds.
- const DakotaIntVector & discrete_lower_bounds () const
  return the active discrete variable lower bounds.
- void discrete_lower_bounds (const DakotaIntVector &d_l_bnds)
  set the active discrete variable lower bounds.
- const DakotaIntVector & discrete_upper_bounds () const
  return the active discrete variable upper bounds.
- void discrete_upper_bounds (const DakotaIntVector &d_u_bnds)
  set the active discrete variable upper bounds.
- void write (ostream &s) const

write a variable constraints object to an ostream.

- void read (istream &s)

  read a variable constraints object from an istream.

Private Attributes

- DakotaRealVector allContinuousLowerBnds

  a continuous lower bounds array combining continuous design, uncertain, and continuous state variable types (all view).

- DakotaRealVector allContinuousUpperBnds

  a continuous upper bounds array combining continuous design, uncertain, and continuous state variable types (all view).

- DakotaIntVector allDiscreteLowerBnds

  a discrete lower bounds array combining discrete design and discrete state variable types (all view).

- DakotaIntVector allDiscreteUpperBnds

  a discrete upper bounds array combining discrete design and discrete state variable types (all view).

- size_t numCDV

  number of continuous design variables.

- size_t numDDV

  number of discrete design variables.

- size_t numUV

  number of uncertain variables.

- size_t numCSV

  number of continuous state variables.

- size_t numDSV

  number of discrete state variables.

6.3.1 Detailed Description

Derived class within the DakotaVarConstraints hierarchy which employs the all data view.

Derived variable constraints classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The AllVarConstraints derived class combines design, uncertain, and state variable types but separates continuous and discrete domain types. The result is combined continuous bounds arrays (allContinuousLowerBnds, allContinuousUpperBnds) and combined discrete bounds arrays (allDiscreteLowerBnds, allDiscreteUpperBnds). Parameter and DACE studies currently use this approach (see DakotaVariables::get_variables(problem_db) for variables type selection; variables type is passed to the DakotaVarConstraints constructor in DakotaModel).

6.3.2 Constructor & Destructor Documentation

6.3.2.1 AllVarConstraints::AllVarConstraints (const ProblemDescDB & *problem_db*)

constructor.

Extract fundamental lower and upper bounds and combine them into allContinuousLowerBnds, allContinuousUpperBnds, allDiscreteLowerBnds, and allDiscreteUpperBnds using utilities from VariablesUtil.

The documentation for this class was generated from the following files:

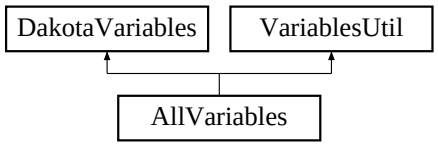
- AllVarConstraints.H
- AllVarConstraints.C

6.4 AllVariables Class Reference

Derived class within the DakotaVariables hierarchy which employs the all data view.

`#include <AllVariables.H>`

Inheritance diagram for AllVariables::



Public Methods

- AllVariables ()
  default constructor.
- AllVariables (const ProblemDescDB &problem_db)
  standard constructor.
- ~AllVariables ()
  destructor.
- size_t tv () const
  Returns total number of vars.
- size_t cv () const
  Returns number of active continuous vars.
- size_t dv () const
  Returns number of active discrete vars.
- const DakotaRealVector & continuous_variables () const
  return the active continuous variables.
- void continuous_variables (const DakotaRealVector &c_vars)
  set the active continuous variables.
- const DakotaIntVector & discrete_variables () const
  return the active discrete variables.
- void discrete_variables (const DakotaIntVector &d_vars)
  set the active discrete variables.
- const DakotaStringArray & continuous_variable_labels () const

return the active continuous variable labels.

- void continuous_variable_labels (const DakotaStringArray &cv_labels)
  set the active continuous variable labels.
- const DakotaStringArray & discrete_variable_labels () const
  return the active discrete variable labels.
- void discrete_variable_labels (const DakotaStringArray &dv_labels)
  set the active discrete variable labels.
- const DakotaRealVector & inactive_continuous_variables () const
  return the inactive continuous variables.
- void inactive_continuous_variables (const DakotaRealVector &i_c_vars)
  set the inactive continuous variables.
- const DakotaIntVector & inactive_discrete_variables () const
  return the inactive discrete variables.
- void inactive_discrete_variables (const DakotaIntVector &i_d_vars)
  set the inactive discrete variables.
- size_t acv () const
  returns total number of continuous vars.
- size_t adv () const
  returns total number of discrete vars.
- DakotaRealVector all_continuous_variables () const
  returns a single array with all continuous variables.
- DakotaIntVector all_discrete_variables () const
  returns a single array with all discrete variables.
- void read (istream &s)
  read a variables object from an istream.
- void write (ostream &s) const
  write a variables object to an ostream.
- void read_annotated (istream &s)
  read a variables object in annotated format from an istream.
- void write_annotated (ostream &s) const
  write a variables object in annotated format to an ostream.
- void read (DakotaBiStream &s)
  read a variables object from the binary restart stream.

- void write (DakotaBoStream &s) const
  write a variables object to the binary restart stream.
- void read (UnPackBuffer &s)
  read a variables object from a packed MPI buffer.
- void write (PackBuffer &s) const
  write a variables object to a packed MPI buffer.

Private Methods

- void copy_rep (const DakotaVariables *vars_rep)
  Used by copy() to copy the contents of a letter class.

Private Attributes

- DakotaRealVector allContinuousVars
  a continuous array combining continuous design, uncertain, and continuous state variable types (all).
- DakotaIntVector allDiscreteVars
  a discrete array combining discrete design and discrete state variable types (all).
- DakotaStringArray allContinuousLabels
  a label array combining continuous design, uncertain, and continuous state variable types (all).
- DakotaStringArray allDiscreteLabels
  a label array combining discrete design and discrete state variable types (all).
- DakotaRealVector emptyRealVector
  an empty real vector returned in get functions when there are no variables corresponding to the request.
- DakotaIntVector emptyIntVector
  an empty int vector returned in get functions when there are no variables corresponding to the request.
- size_t numCDV
  number of continuous design variables.
- size_t numDDV
  number of discrete design variables.
- size_t numUV
  number of uncertain variables.
- size_t numCSV
  number of continuous state variables.
- size_t numDSV
  number of discrete state variables.

Friends

- int operator== (const AllVariables &vars1, const AllVariables &vars2)

  equality operator.

6.4.1 Detailed Description

Derived class within the DakotaVariables hierarchy which employs the all data view.

Derived variables classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The AllVariables derived class combines design, uncertain, and state variable types but separates continuous and discrete domain types. The result is a single array of continuous variables (allContinuousVars) and a single array of discrete variables (allDiscreteVars). Parameter and DACE studies currently use this approach (see DakotaVariables::get_variables(problem_db)).

6.4.2 Constructor & Destructor Documentation

6.4.2.1 AllVariables::AllVariables (const ProblemDescDB & *problem_db*)

standard constructor.

Extract fundamental variable types and labels and combine them into allContinuousVars, allDiscreteVars, allContinuousLabels, and allDiscreteLabels using utilities from VariablesUtil.

The documentation for this class was generated from the following files:

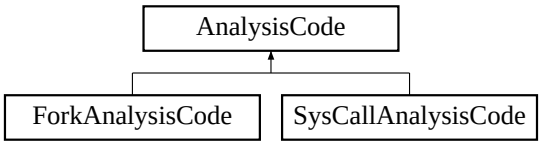
- AllVariables.H
- AllVariables.C

6.5 AnalysisCode Class Reference

Base class providing common functionality for derived classes (SysCallAnalysisCode and ForkAnalysisCode) which spawn separate processes for managing simulations.

`#include <AnalysisCode.H>`

Inheritance diagram for AnalysisCode::



Public Methods

- void define_filenames (const int id)
  define modified filenames from user input by handling Unix temp file and tagging options.
- void write_parameters_file (const DakotaVariables &vars, const DakotaIntArray &asv, const int id)
  write the variables and active set vector objects to the parameters file in either standard or aprepro format.
- void read_results_file (DakotaResponse &response, const int id)
  read the response object from the results file.
- const DakotaStringList & program_names () const
  return programNames.
- const DakotaString & input_filter_name () const
  return iFilterName.
- const DakotaString & output_filter_name () const
  return oFilterName.
- const DakotaString & modified_parameters_filename () const
  return modifiedParamsFileName.
- const DakotaString & modified_results_filename () const
  return modifiedResFileName.
- const DakotaString & results_fname (const int id) const
  return the entry in resultsFNameList corresponding to id.
- void quiet_flag (const short flag)
  set quietFlag.

- short quiet_flag () const

  return quietFlag.

Protected Methods

- AnalysisCode (const ProblemDescDB &problem_db)

  constructor.

- virtual ~AnalysisCode ()

  destructor.

Protected Attributes

- short quietFlag

  flag set by master processor to quiet output from slave processors.

- short verboseFlag

  flag for additional analysis code output if method verbosity is set.

- short fileTagFlag

  flags tagging of parameter/results files.

- short fileSaveFlag

  flags retention of parameter/results files.

- short apreproFlag

  flags use of the APREPRO (the Sandia "A PRE PROcessor" utility) format for parameter files.

- DakotaString iFilterName

  the name of the input filter (input_filter user specification).

- DakotaString oFilterName

  the name of the output filter (output_filter user specification).

- DakotaStringList programNames

  the names of the analysis code programs (analysis_drivers user specification).

- size_t numPrograms

  the number of analysis code programs (length of programNames list).

- DakotaString parametersFileName

  the name of the parameters file from user specification.

- DakotaString modifiedParamsFileName

  the parameters file name actually used (modified with tagging or temp files).

- DakotaString resultsFileName

the name of the results file from user specification.

- DakotaString modifiedResFileName

  the results file name actually used (modified with tagging or temp files).

- DakotaStringList parametersFNameList

  list of parameters file names used in spawning function evaluations.

- DakotaStringList resultsFNameList

  list of results file names used in spawning function evaluations.

- DakotaIntList fileNameKey

  stores function evaluation identifiers to allow key-based retrieval of file names from parametersFNameList and resultsFNameList.

Private Attributes

- ParallelLibrary & parallelLib

  reference to the ParallelLibrary object. Used in define_filenames().

6.5.1 Detailed Description

Base class providing common functionality for derived classes (SysCallAnalysisCode and ForkAnalysisCode) which spawn separate processes for managing simulations.

The AnalysisCode class hierarchy provides simulation spawning services for ApplicationInterface derived classes and alleviates these classes of some of the specifics of simulation code management. The hierarchy does not employ the letter-envelope technique since the ApplicationInterface derived classes instantiate the appropriate derived AnalysisCode class directly.

The documentation for this class was generated from the following files:

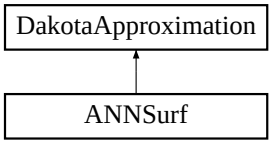
- AnalysisCode.H
- AnalysisCode.C

6.6 ANNSurf Class Reference

Derived approximation class for artificial neural networks.

`#include <ANNSurf.H>`

Inheritance diagram for ANNSurf::



Public Methods

- ANNSurf (const ProblemDescDB &problem_db)

  constructor.

- ~ANNSurf ()

  destructor.

Protected Methods

- int required_samples (int num_vars)

  return the minimum number of samples required to build the derived class approximation type in num_vars dimensions.

- void find_coefficients ()

  calculate the data fit coefficients using the currentPoints list of SurrogateDataPoints.

- Real get_value (const DakotaRealVector &x)

  retrieve the approximate function value for a given parameter vector.

Private Attributes

- ANNApprox * annObject

  pointer to the ANNApprox object (see VendorPackages/ann for class declaration).

6.6.1 Detailed Description

Derived approximation class for artificial neural networks.

The ANNSurf class uses a layered-perceptron artificial neural network. Unlike most neural networks, it does not employ a back-propagation approach to training. Rather it uses a direct training approach developed by Prof. David Zimmerman of the University of Houston and modified by Tom Paez and Chris O'Gorman of Sandia. It is more computationally efficient that back-propagation networks, but relative accuracy can be a concern.

The documentation for this class was generated from the following files:

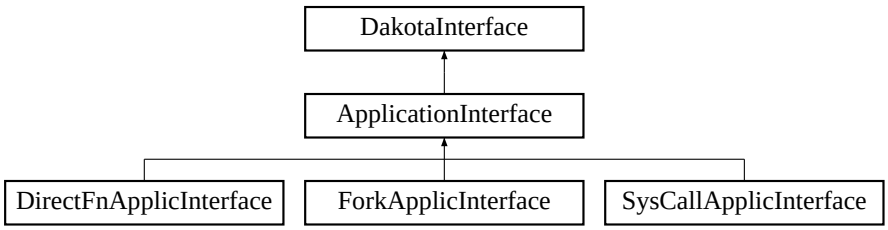
- ANNSurf.H
- ANNSurf.C

6.7 ApplicationInterface Class Reference

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

`#include <ApplicationInterface.H>`

Inheritance diagram for ApplicationInterface::



Protected Methods

- ApplicationInterface (const ProblemDescDB &problem_db, const size_t &num_fns)

  constructor.

- ~ApplicationInterface ()

  destructor.

- void init_communicators (const DakotaIntArray &message_lengths, const int &max_iterator_concurrency)

  allocate communicators for the evaluation and analysis parallelism levels.

- void free_communicators ()

  deallocate communicators for the evaluation and analysis parallelism levels.

- int asynch_local_evaluation_concurrency () const

  return asynchLocalEvalConcurrency.

- DakotaString interface_synchronization () const

  return interfaceSynchronization.

- void map (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response, const int asynch_flag=0)

  Provides a "mapping" of variables to responses using a simulation. Protected due to DakotaInterface letter-envelope idiom.

- void manage_failure (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response, int failed_eval_id)

  manages a simulation failure using abort/retry/recover/continuation.

- const DakotaArray< DakotaResponse > & synch ()

executes a blocking schedule for asynchronous evaluations in the beforeSynchPRPList queue and returns all jobs.

- const DakotaList< DakotaResponse > & synch_nowait ()

  executes a nonblocking schedule for asynchronous evaluations in the beforeSynchPRPList queue and returns a partial list 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.

- virtual void derived_map (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response, int fn_eval_id)=0

  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)=0

  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 derived_synch (DakotaList< ParamResponsePair > &prp_list)=0

  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 derived_synch_nowait (DakotaList< ParamResponsePair > &prp_list)=0

  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 clear_bookkeeping ()

  clears any bookkeeping in derived classes.

- void self_schedule_analyses ()

  blocking self-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 derived_synchronous_local_analysis (const int &analysis_id)=0

  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.

- short evalMessagePass

  flags use of message passing at the level of evaluation scheduling.

- short analysisMessagePass

  flags use of message passing at the level of analysis scheduling.

- short suppressOutput

  flag for suppressing output on slave processors.

- int asynchLocalAnalysisConcurrency

  limits the number of concurrent analyses in asynchronous local scheduling and specifies hybrid concurrency when message passing.

- short asynchLocalAnalysisFlag

  flag for asynchronous local parallelism of analyses.

- int worldSize

  size of MPI_COMM_WORLD.

- int iteratorCommSize

  size of iteratorComm.

- int evalCommSize

  size of evalComm.

- int analysisCommSize

  size of analysisComm.

- int worldRank

  processor rank within MPI_COMM_WORLD.

- int iteratorCommRank

  processor rank within iteratorComm.

- int evalCommRank

  processor rank within evalComm.

- int analysisCommRank

  processor rank within analysisComm.

- int evalServerId

  evaluation server identifier.

- int analysisServerId

  analysis server identifier.

- short evalDedMasterFlag

  flag for dedicated master partitioning at the level of evaluation scheduling.

- short multiProcAnalysisFlag

  flag for multiprocessor analysis partitions.

- DakotaStringList analysisDrivers

  the set of analyses within each function evaluation (from the analysis_drivers interface specification).

- int numAnalysisDrivers

  length of analysisDrivers list.

- int numAnalysisServers

  number of analysis servers.

- MPI_Comm evalComm

  intracomm for fn eval; partition of iteratorComm.

- MPI_Comm analysisComm

  intracomm for analysis; partition of evalComm.

- int lenVarsMessage

  length of a PackBuffer containing a DakotaVariables object; computed in DakotaModel::init_communicators().

- int lenVarsASVMessage

  length of a PackBuffer containing a DakotaVariables object and an active set vector object; computed in DakotaModel::init_communicators().

- int lenResponseMessage

  length of a PackBuffer containing a DakotaResponse object; computed in DakotaModel::init_communicators().

- int lenPRPairMessage

  length of a PackBuffer containing a ParamResponsePair object; computed in DakotaModel::init_communicators().

Private Methods

- int duplication_detect (const DakotaVariables &vars, DakotaResponse &response, const int asynch_flag)

  checks data_pairs and beforeSynchPRPList to see if the current evaluation request has already been performed or queued.

- void self_schedule_evaluations ()

  blocking self-schedule of all evaluations in beforeSynchPRPList using message passing; executes on iteratorComm master.

- void static_schedule_evaluations ()

  blocking static schedule of all evaluations in beforeSynchPRPList using message passing; executes on iteratorComm master.

- void asynchronous_local_evaluations (DakotaList< ParamResponsePair > &prp_list)

perform all jobs in prp_list using asynchronous approaches on the local processor.

- void synchronous_local_evaluations (DakotaList< ParamResponsePair > &prp_list)

  perform all jobs in prp_list using synchronous approaches on the local processor.

- void asynchronous_local_evaluations_nowait (DakotaList< ParamResponsePair > &prp_list)

  launch new jobs in prp_list asynchronously (if capacity is available), perform nonblocking query of all running jobs, and process any completed jobs.

- void serve_evaluations_synch ()

  serve the evaluation message passing schedulers and perform one synchronous evaluation at a time.

- void serve_evaluations_asynch ()

  serve the evaluation message passing schedulers and manage multiple asynchronous evaluations.

- void serve_evaluations_peer ()

  serve the evaluation message passing schedulers and perform one synchronous evaluation at a time as part of the 1st peer.

- const ParamResponsePair & get_source_pair (const DakotaVariables &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 DakotaVariables &target_vars, const DakotaIntArray &asv, DakotaResponse &response, const ParamResponsePair &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".

Private Attributes

- int numEvalServers

  number of evaluation servers.

- int procsPerAnalysis

  processors per analysis servers.

- DakotaString evalScheduling

  user specification of evaluation scheduling algorithm (self, static, or no spec). Used for manual overrides of the auto-configure logic in ParallelLibrary::resolve_inputs().

- DakotaString analysisScheduling

  user specification of analysis scheduling algorithm (self, static, or no spec). 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.

- DakotaString interfaceSynchronization

  interface synchronization specification: synchronous (default) or asynchronous.

- short headerFlag

  used by synch_nowait to manage output frequency (since this function may be called many times prior to any completions).

- short asvControl

  used by map to manage the user's setting for active set vector control. 1 = on = modify the ASV each evaluation as appropriate (default); 0 = off = ASV values are static so that the user need not check them on each evaluation.

- DakotaIntArray defaultASV

  the static ASV values used when the user has selected asvControl = off.

- DakotaString failAction

  mitigation action for captured simulation failures: abort, retry, recover, or continuation.

- int failRetryLimit

  limit on the number of retries for the retry failAction.

- DakotaRealVector failRecoveryFnVals

  the dummy function values used for the recover failAction.

- DakotaIntList historyDuplicateIds

  used to bookkeep fnEvalId of asynchronous evaluations which duplicate data_pairs evaluations.

- DakotaList< DakotaResponse > historyDuplicateResponses

  used to bookkeep response of asynchronous evaluations which duplicate data_pairs evaluations.

- DakotaIntList beforeSynchDuplicateIds

  used to bookkeep fnEvalId of asynchronous evaluations which duplicate queued beforeSynchPRPList evaluations.

- DakotaSizetList beforeSynchDuplicateIndices

  used to bookkeep beforeSynchPRPList index of asynchronous evaluations which duplicate queued beforeSynchPRPList evaluations.

- DakotaList< DakotaResponse > beforeSynchDuplicateResponses

  used to bookkeep response of asynchronous evaluations which duplicate queued beforeSynchPRPList evaluations.

- DakotaIntList runningList

  used by asynchronous_local_nowait to bookkeep which jobs are running.

- DakotaList< ParamResponsePair > beforeSynchPRPList

  used to bookkeep vars/asv/response of nonduplicate asynchronous evaluations. This is the queue of jobs populated by asynchronous map() invocations which is later scheduled on a call to synch() or synch_nowait().

6.7.1 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 XML over sockets.

6.7.2 Member Function Documentation

6.7.2.1 void ApplicationInterface::map (const DakotaVariables & *vars*, const DakotaIntArray & *asv*, DakotaResponse & *response*, const int *asynch_flag* = 0) [protected, virtual]

Provides a "mapping" of variables to responses using a simulation. Protected due to DakotaInterface letter-envelope idiom.

The function evaluator for application interfaces. Called from derived_compute_response() and derived_asynch_compute_response() in derived DakotaModel classes. If asynch_flag is not set, perform a blocking evaluation (using derived_map()). If asynch_flag is set, add the job to the beforeSynchPRPList queue for execution by one of the scheduler routines in synch() or synch_nowait(). Duplicate function evaluations are detected with duplication_detect().

Reimplemented from DakotaInterface.

6.7.2.2 const DakotaArray< DakotaResponse > & ApplicationInterface::synch () [protected, virtual]

executes a blocking schedule for asynchronous evaluations in the beforeSynchPRPList queue 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 DakotaModel classes.

Reimplemented from DakotaInterface.

6.7.2.3 const DakotaList< DakotaResponse > & ApplicationInterface::synch_nowait () [protected, virtual]

executes a nonblocking schedule for asynchronous evaluations in the beforeSynchPRPList queue and returns a partial list of completed jobs.

This function will eventually provide nonblocking synchronization for all cases of asynchronous evaluations, however it currently supports only the local asynchronous case since nonblocking message passing schedulers have not yet been implemented. Called from derived_synchronize_nowait() in derived DakotaModel classes.

Reimplemented from DakotaInterface.

6.7.2.4 void ApplicationInterface::serve_evaluations () [protected, virtual]

run on evaluation servers to serve the iterator master.

Invoked by the serve() function in derived DakotaModel classes. Passes control to serve_evaluations_asynch(), serve_evaluations_peer(), or serve_evaluations_synch() according to specified concurrency and self/static scheduler configuration.

Reimplemented from DakotaInterface.

6.7.2.5 void ApplicationInterface::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 both USE_MPI and iteratorCommSize to provide appropriate fall through behavior.

Reimplemented from DakotaInterface.

6.7.2.6 void ApplicationInterface::self_schedule_analyses () [protected]

blocking self-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 self-scheduling of analyses among slave servers. It is patterned after self_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. Self-scheduling approach 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.

6.7.2.7 void ApplicationInterface::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().

6.7.2.8 int ApplicationInterface::duplication_detect (const DakotaVariables & *vars*, DakotaResponse & *response*, const int *asynch_flag*) [private]

checks data_pairs and beforeSynchPRPList to see if the current evaluation request has already been performed or queued.

Check incoming evaluation request for duplication with content of data_pairs and beforeSynchPRPList. If duplication is detected, return true, else return false. Manage bookkeeping with historyDuplicate and beforeSynchDuplicate lists. Called from map().

6.7.2.9 void ApplicationInterface::self_schedule_evaluations () [private]

blocking self-schedule of all evaluations in beforeSynchPRPList using message passing; executes on iteratorComm master.

This code is called from synch() to provide the master portion of a master-slave algorithm for the dynamic self-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. Self-scheduling approach 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.

6.7.2.10 void ApplicationInterface::static_schedule_evaluations () [private]

blocking static schedule of all evaluations in beforeSynchPRPList using message passing; executes on iteratorComm master.

This code runs on the iteratorCommRank 0 processor (the iterator) and is called from synch() in order to assign a static schedule. It matches serve_evaluations_peer() for any other processors within the 1st evaluation partition and serve_evaluations_synch()/serve_evaluations_asynch() for all other evaluation partitions (depending on asynchLocalEvalConcurrency). It performs function evaluations locally for its portion of the static schedule 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 beforeSynchPRPList (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.

6.7.2.11 void ApplicationInterface::asynchronous_local_evaluations (DakotaList< ParamResponsePair > & *prp_list*) [private]

perform all jobs in prp_list 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 synch() for a complete local scheduling of all asynchronous jobs or from static_schedule_evaluations() to perform a local portion of the total job set. It uses the derived_map_asynch() to initiate asynchronous evaluations and derived_synch() to capture completed jobs, and mirrors the self_schedule_evaluations() message passing scheduler as much as possible (derived_synch() is modeled after MPI_Waitsome()).

6.7.2.12 void ApplicationInterface::synchronous_local_evaluations (DakotaList< ParamResponsePair > & *prp_list*) [private]

perform all jobs in prp_list 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 static_schedule_evaluations() to perform a local portion of the total job set.

6.7.2.13 void ApplicationInterface::asynchronous_local_evaluations_nowait (DakotaList< ParamResponsePair > & *prp_list*) [private]

launch new jobs in prp_list asynchronously (if capacity is available), perform nonblocking query of all running jobs, and process any completed jobs.

This function provides nonblocking synchronization for the local asynch case (background system call, nonblocking fork, or threads). It is called from synch_nowait() and passed the complete set of all asynchronous jobs (beforeSynchPRPList). It uses derived_map_asynch() to initiate asynchronous evaluations and derived_synch_nowait() to capture completed jobs in nonblocking mode. It mirrors a nonblocking message passing scheduler as much as possible (derived_synch_nowait() modeled after MPI_Testsome()). The results of this function are rawResponseList and completionList. Since rawResponseList is in no particular order, completionList must be used as a key. It is assumed that the incoming prp_list contains only active and new jobs - i.e., all completed jobs are cleared by synch_nowait().

6.7.2.14 void ApplicationInterface::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()).

6.7.2.15 void ApplicationInterface::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).

6.7.2.16 void ApplicationInterface::serve_evaluations_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 the bcast() in synchronous_local_evaluations(), which is invoked by static_schedule_evaluations()).

The documentation for this class was generated from the following files:

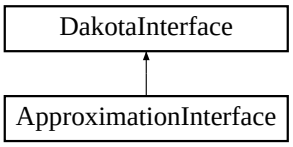
- ApplicationInterface.H
- ApplicationInterface.C

6.8 ApproximationInterface Class Reference

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

`#include <ApproximationInterface.H>`

Inheritance diagram for ApproximationInterface::



Public Methods

- ApproximationInterface (ProblemDescDB &problem_db, const size_t &num_acv, const size_t &num_fns)

  constructor.

- ~ApproximationInterface ()

  destructor.

Protected Methods

- void map (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response, const int asynch_flag=0)

  the function evaluator: provides an approximate "mapping" from the variables to the responses using functionSurfaces.

- int minimum_samples () const

  returns minSamples.

- void build_global_approximation (DakotaIterator &dace_iterator)

  builds a global approximation for use as a surrogate.

- void build_local_approximation (DakotaModel &actual_model)

  builds a local approximation for use as a surrogate.

- void update_approximation (const DakotaRealVector &x_star, const DakotaResponse &response_star)

  updates an existing global approximation with new data.

- const DakotaArray< DakotaResponse > & synch ()

  recovers data from a series of asynchronous evaluations (blocking).

- const DakotaList< DakotaResponse > & synch_nowait ()

  recovers data from a series of asynchronous evaluations (nonblocking).

Private Attributes

- DakotaString daceMethodPointer

  string pointer to the dace iterator specified by the user in the global approximation specification.

- DakotaString actualInterfacePointer

  string pointer to the actual interface specified by the user in the local/multipoint approximation specifications.

- DakotaArray< DakotaApproximation > functionSurfaces

  list of approximations, one per response function.

- DakotaRealVector approxScale

  vector of approximation scalings from an external file.

- DakotaRealVector approxOffset

  vector of approximation offsets from an external file.

- DakotaString sampleReuse

  user selection of sample reuse type: all, region, or none (default).

- short graphicsFlag

  controls 3D graphics of approximation surfaces.

- int minSamples

  the minimum number of samples over all functionSurfaces.

- DakotaList< DakotaResponse > beforeSynchResponseList

  bookkeeping list to catalogue responses generated in map for use in synch() and synch_nowait(). This supports pseudo-asynchronous operations (approximate responses all always computed synchronously, but asynchronous virtual functions are supported through bookkeeping).

6.8.1 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 DakotaApproximation objects, one for each response function.

6.8.2 Member Data Documentation

6.8.2.1 DakotaString ApproximationInterface::daceMethodPointer [private]

string pointer to the dace iterator specified by the user in the global approximation specification.

This pointer is *not* used for building objects since this is managed in SurrLayeredModels. Its use in ApproximationInterface is currently limited to flagging dace contributions to data sets in build_global_approximation().

6.8.2.2 DakotaString ApproximationInterface::actualInterfacePointer [private]

string pointer to the actual interface specified by the user in the local/multipoint approximation specifications.

This pointer is *not* used for building objects since this is managed in SurrLayeredModels. Its use in ApproximationInterface is currently limited to header output.

6.8.2.3 DakotaArray<DakotaApproximation> ApproximationInterface::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.

The documentation for this class was generated from the following files:

- ApproximationInterface.H
- ApproximationInterface.C

6.9 BaseConstructor Struct Reference

Dummy struct for overloading letter-envelope constructors.

`#include <ProblemDescDB.H>`

Public Methods

- BaseConstructor (int=0)

  C++ structs can have constructors.

6.9.1 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 (rather than in a header of a class that uses it) avoids problems with circular dependencies.

The documentation for this struct was generated from the following file:

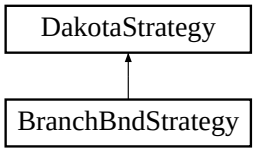
- ProblemDescDB.H

6.10 BranchBndStrategy Class Reference

Strategy for mixed integer nonlinear programming using the PICO parallel branch and bound engine.

`#include <BranchBndStrategy.H>`

Inheritance diagram for BranchBndStrategy::



Public Methods

- BranchBndStrategy (ProblemDescDB &problem_db)

  constructor.

- ~BranchBndStrategy ()

  destructor.

- void run_strategy ()

  Performs the branch and bound strategy by executing selectedIterator on userDefinedModel multiple times in parallel for different variable bounds within the model.

Private Attributes

- DakotaModel userDefinedModel

  the model used by the iterator.

- DakotaIterator selectedIterator

  the iterator used by BranchBndStrategy.

- int numIteratorServers

  number of concurrent iterator partitions.

- int numRootSamples

  number of samples to perform at the root of the branching structure.

- int numNodeSamples

  number of samples to perform at each node of the branching structure.

- MPI_Comm picoComm

  MPI intracommunicator for PICO hub processors (strategy and iterator masters).

- int picoCommRank

  processor rank in picoComm.

- int picoCommSize

  number of processors in picoComm.

- int argC

  dummy argument count passed to pico classes in init(), readAll(), and readAndBroadcast().

- char ** argV

  dummy argument vector passed to pico classes in init(), readAll(), and readAndBroadcast().

- DoubleVector picoLowerBnds

  global lower bounds for merged continuous & discrete design variables passed to PICO (copied from userDefinedModel).

- DoubleVector picoUpperBnds

  global upper bounds for merged continuous & discrete design variables passed to PICO (copied from userDefinedModel).

- IntVector picoListOfIntegers

  key to the discrete variables which have been relaxed and merged into the continuous variables and bounds arrays (indices in the combined arrays).

6.10.1 Detailed Description

Strategy for mixed integer nonlinear programming using the PICO parallel branch and bound engine.

This strategy combines the PICO branching engine with nonlinear programming optimizers from DAKOTA (e.g., DOT, NPSOL, OPT++) to solve mixed integer nonlinear programs. The discrete variables in the problem must support relaxation, i.e., they must be able to assume nonintegral values during the solution process. PICO selects solution ”branches”, each of which constrains the problem to lie within different variable bounds. The series of branches selected is designed to drive integer variables to their integral values. For each of the branches, a nonlinear DAKOTA optimizer is used to solve the optimization problem and return the solution to PICO. If this solution has all of the integer variables at integral values, then it provides an upper bound on the true solution. This bound can be used to prune other branches, since there is no need to further investigate a branch which does not yet have integral values for the integer variables and which has an objective function worse than the bound. In linear programs, the bounding and pruning processes are rigorous and will lead to the exact global optimum. In nonlinear problems, the bounding and pruning processes are heuristic, i.e. they will find local optima but the global optimum may be missed. PICO supports parallelism between ”hubs,” each of which drives a concurrent iterator partition in DAKOTA (and each of these iterator partitions may have lower levels of nested parallelism). This complexity is hidden from PICO through the use of picoComm, which contains the set of master iterator processors, one from each iterator partition. Thus, PICO can schedule jobs among single-processor hubs in its normal manner, unaware of the nested parallelism complexities that may occur within each nonlinear optimization.

The documentation for this class was generated from the following files:

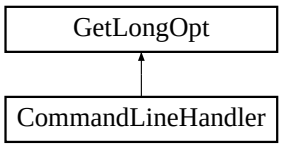
- BranchBndStrategy.H
- BranchBndStrategy.C

6.11 CommandLineHandler Class Reference

Utility class for managing command line inputs to DAKOTA.

`#include <CommandLineHandler.H>`

Inheritance diagram for CommandLineHandler::



Public Methods

- CommandLineHandler ()
  constructor.
- ~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.
- const char * read_restart_stream ()
  Returns the filename of the restart file as specified on the DAKOTA command line.
- const char * write_restart_stream ()
  Returns the filename of the restart file as specified on the DAKOTA command line.
- int read_restart_evals ()
  Returns the number of evaluations to be read from the restart file as specified on the DAKOTA command line.

6.11.1 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.

The documentation for this class was generated from the following files:

- CommandLineHandler.H
- CommandLineHandler.C

6.12 CommandShell Class Reference

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

`#include <CommandShell.H>`

Public Methods

- CommandShell ()
  constructor.
- ~CommandShell ()
  destructor.
- CommandShell & operator<< (const char *string)
  adds string to unixCommand.
- CommandShell & operator<< (CommandShell &(*f)(CommandShell &))
  allows passing of the flush function to the shell using <<.
- CommandShell & flush ()
  "flushes" the shell; i.e. executes the unixCommand.
- void asynch_flag (const short flag)
  set the asynchFlag.
- short asynch_flag () const
  get the asynchFlag.
- void quiet_flag (const short flag)
  set the quietFlag.
- short quiet_flag () const
  get the quietFlag.

Private Attributes

- DakotaString unixCommand
  the command string that is constructed through one or more << insertions and then executed by flush.
- short asynchFlag
  flags nonblocking operation (background system calls).
- short quietFlag
  flags quiet operation (no command echo).

6.12.1 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.

6.12.2 Member Function Documentation

6.12.2.1 CommandShell & CommandShell::flush ()

"flushes" the shell; i.e. executes the unixCommand.

Executes the unixCommand by passing it to system(). Appends an "&" if asynchFlag is set (background system call) and echos the unixCommand to cout if quietFlag is not set.

The documentation for this class was generated from the following files:

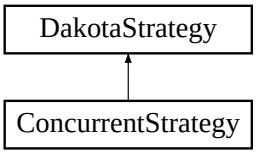
- CommandShell.H
- CommandShell.C

6.13 ConcurrentStrategy Class Reference

Strategy for multi-start iteration or pareto set optimization.

`#include <ConcurrentStrategy.H>`

Inheritance diagram for ConcurrentStrategy::



Public Methods

- ConcurrentStrategy (ProblemDescDB &problem_db)

  constructor.

- ~ConcurrentStrategy ()

  destructor.

- void run_strategy ()

  Performs the concurrent strategy by executing selectedIterator on userDefinedModel multiple times in parallel for different settings within the iterator or model.

Private Attributes

- DakotaModel userDefinedModel

  the model used by the iterator.

- DakotaIterator selectedIterator

  the iterator used by the concurrent strategy.

- int numIteratorServers

  number of concurrent iterator partitions.

- int numIteratorJobs

  total number of iterator executions to schedule over the servers.

- DakotaRealVectorArray iteratorParameterSets

  an array of parameter set vectors (either multistart variable sets or pareto multiobjective weighting sets) to be performed.

- short strategyDedicatedMasterFlag

  signals ded. master partitioning.

- int iteratorServerId

  identifier for an iterator server.

6.13.1 Detailed Description

Strategy for multi-start iteration or pareto set optimization.

This strategy 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 mutiobjective formulations) is provided. This pareto set is mapped through running an optimizer multiple times for different sets of multiobjective weightings.

The documentation for this class was generated from the following files:

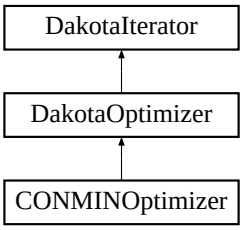
- ConcurrentStrategy.H
- ConcurrentStrategy.C

6.14 CONMINOptimizer Class Reference

Wrapper class for the CONMIN optimization library.

`#include <CONMINOptimizer.H>`

Inheritance diagram for CONMINOptimizer::



Public Methods

- CONMINOptimizer (DakotaModel &model)

  constructor.

- ~CONMINOptimizer ()

  destructor.

- void find_optimum ()

  Used within the optimizer branch for computing the optimal solution. Redefines the run_iterator virtual function for the optimizer branch.

Private Methods

- void allocate_workspace ()

  Allocates workspace for the optimizer.

Private Attributes

- int conminInfo

  INFO from CONMIN manual.

- int printControl

  IPRINT from CONMIN manual (controls output verbosity).

- int optimizationType

  MINMAX from DOT manual (minimize or maximize).

- DakotaRealVector localConstraintValues

  array of nonlinear constraint values passed to CONMIN.

- DakotaSizetList constraintMappingIndices

  a list of indices for referencing the corresponding DakotaResponse constraints used in computing the CONMIN constraints.

- DakotaRealList constraintMappingMultipliers

  a list of multipliers for mapping the DakotaResponse constraints to the CONMIN constraints.

- DakotaRealList constraintMappingOffsets

  a list of offsets for mapping the DakotaResponse constraints to the CONMIN constraints.

- 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.

- Real FDCH

  Relative finite difference step size.

- Real FDCHM

  Absolute finite difference step size.

- Real CT

  Constraint thickness parameter.

- Real CTMIN

  Minimum absolute value of CT used during optimization.

- Real CTL

Constraint thickness parameter for linear and side constraints.

- Real CTLMIN

  Minimum value of CTL used during optimization.

- Real DELFUN

  Relative convergence criterion threshold.

- Real DABFUN

  Absolute convergence criterion threshold.

- Real * conminDesVars

  Array of design variables used by CONMIN (length N1 = numdv+2).

- Real * conminLowerBnds

  Array of lower bounds used by CONMIN (length N1 = numdv+2).

- Real * conminUpperBnds

  Array of upper bounds used by CONMIN (length N1 = numdv+2).

- Real * S

  Internal CONMIN array.

- Real * G1

  Internal CONMIN array.

- Real * G2

  Internal CONMIN array.

- Real * B

  Internal CONMIN array.

- Real * C

  Internal CONMIN array.

- int * MS1

  Internal CONMIN array.

- Real * SCAL

  Internal CONMIN array.

- Real * DF

  Internal CONMIN array.

- Real * A

  Internal CONMIN array.

- int * ISC

  Internal CONMIN array.

- int * IC

  Internal CONMIN array.

6.14.1 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 function and static attribute issues that arise with function pointer designs (see NPSOLOptimizer and SNLLOptimizer).

The user input mappings are as follows: `max_iterations` is mapped into CONMIN's `ITMAX` parameter, `max_function_evaluations` is implemented directly in the find_optimum() 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.

6.14.2 Member Data Documentation

6.14.2.1 int CONMINOptimizer::conminInfo [private]

INFO from CONMIN manual.

Information requested by CONMIN: 1 = evaluate objective and constraints, 2 = evaluate gradients of objective and constraints.

6.14.2.2 int CONMINOptimizer::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

6.14.2.3 int CONMINOptimizer::optimizationType [private]

MINMAX from DOT manual (minimize or maximize).

Values of 0 or -1 (minimize) or 1 (maximize).

6.14.2.4 DakotaRealVector CONMINOptimizer::localConstraintValues [private]

array of nonlinear constraint values passed to CONMIN.

This array must be of nonzero length (sized with localConstraintArraySize) and must contain only one-sided inequality constraints which are <= 0 (which requires a transformation from 2-sided inequalities and equalities).

6.14.2.5 DakotaSizetList CONMINOptimizer::constraintMappingIndices [private]

a list of indices for referencing the corresponding DakotaResponse constraints used in computing the CONMIN constraints.

The length of the list corresponds to the number of CONMIN constraints, and each entry in the list points to the corresponding DAKOTA constraint.

6.14.2.6 DakotaRealList CONMINOptimizer::constraintMappingMultipliers [private]

a list of multipliers for mapping the DakotaResponse constraints to the CONMIN constraints.

The length of the list corresponds to the number of CONMIN constraints, and each entry in the list contains a multiplier for the DAKOTA constraint identified with constraintMappingIndices. These multipliers are currently +1 or -1.

6.14.2.7 DakotaRealList CONMINOptimizer::constraintMappingOffsets [private]

a list of offsets for mapping the DakotaResponse constraints to the CONMIN constraints.

The length of the list corresponds to the number of CONMIN constraints, and each entry in the list contains an offset for the DAKOTA constraint identified with constraintMappingIndices. These offsets involve inequality bounds or equality targets, since CONMIN assumes constraint allowables = 0.

6.14.2.8 int CONMINOptimizer::N1 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N1 = number of variables + 2

6.14.2.9 int CONMINOptimizer::N2 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N2 = number of constraints + 2*(number of variables)

6.14.2.10 int CONMINOptimizer::N3 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N3 = Maximum possible number of active constraints.

6.14.2.11 int CONMINOptimizer::N4 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N4 = Maximum(N3,number of variables)

6.14.2.12 int CONMINOptimizer::N5 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N5 = 2∗(N4)

6.14.2.13 Real CONMINOptimizer::CT [private]

Constraint thickness parameter.

The value of CT decreases in magnitude during optimization.

6.14.2.14 Real∗ CONMINOptimizer::S [private]

Internal CONMIN array.

Move direction in N-dimensional space.

6.14.2.15 Real∗ CONMINOptimizer::G1 [private]

Internal CONMIN array.

Temporary storage of constraint values.

6.14.2.16 Real∗ CONMINOptimizer::G2 [private]

Internal CONMIN array.

Temporary storage of constraint values.

6.14.2.17 Real∗ CONMINOptimizer::B [private]

Internal CONMIN array.

Temporary storage for computations involving array S.

6.14.2.18 Real∗ CONMINOptimizer::C [private]

Internal CONMIN array.

Temporary storage for use with arrays B and S.

6.14.2.19 int∗ CONMINOptimizer::MS1 [private]

Internal CONMIN array.

Temporary storage for use with arrays B and S.

6.14.2.20 Real∗ CONMINOptimizer::SCAL [private]

Internal CONMIN array.

Vector of scaling parameters for design parameter values.

6.14.2.21 Real* CONMINOptimizer::DF [private]

Internal CONMIN array.

Temporary storage for analytic gradient data.

6.14.2.22 Real* CONMINOptimizer::A [private]

Internal CONMIN array.

Temporary 2-D array for storage of constraint gradients.

6.14.2.23 int* CONMINOptimizer::ISC [private]

Internal CONMIN array.

Array of flags to identify linear constraints. (not used in this implementation of CONMIN)

6.14.2.24 int* CONMINOptimizer::IC [private]

Internal CONMIN array.

Array of flags to identify active and violated constraints

The documentation for this class was generated from the following files:

- CONMINOptimizer.H
- CONMINOptimizer.C

6.15 CtelRegexp Class Reference

`#include <CtelRegExp.H>`

Public Types

- enum RStatus { **GOOD** = 0, **EXP_TOO_BIG**, **OUT_OF_MEM**, **TOO_MANY_PAR**, **UNMATCH_PAR**, **STARPLUS_EMPTY**, **STARPLUS_NESTED**, **INDEX_RANGE**, **INDEX_MATCH**, **STARPLUS_NOTHING**, **TRAILING**, **INT_ERROR**, **BAD_PARAM**, **BAD_OPCODE** }

  Error codes reported by the engine - Most of these codes never really occurs with this implementation.

Public Methods

- CtelRegexp (const std::string &pattern)

  Constructor - compile a regular expression.

- ~CtelRegexp ()

  Destructor.

- bool compile (const std::string &pattern)

  Compile a new regular expression.

- std::string match (const std::string &str)

  matches a particular string; this method returns a string that is a sub-string matching with the regular expression.

- bool match (const std::string &str, size_t *start, size_t *size)

  another form of matching; returns the indexes of the maching.

- RStatus getStatus ()

  Get status.

- const std::string & getStatusMsg ()

  Get status message.

- void clearErrors ()

  Clear all errors.

- const std::string & getRe ()

  Return regular expression pattern.

- bool split (const std::string &str, std::vector< std::string > &all_matches)

  Split.

Private Methods

- CtelRegexp (const CtelRegexp &)

  Private copy constructor.

- CtelRegexp & operator= (const CtelRegexp &)

  Private assignment operator.

Private Attributes

- std::string strPattern

  STL string to hold pattern.

- regexp * r

  Pointer to regexp.

- RStatus status

  Return status, enumerated type.

- std::string statusMsg

  STL string to hold status message.

6.15.1 Detailed Description

DESCRIPTION: Wrapper for the Regular Expression engine(regexp) released by Henry Spencer of the University of Toronto.

The documentation for this class was generated from the following files:

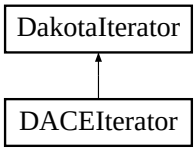
- CtelRegExp.H
- CtelRegExp.C

6.16 DACEIterator Class Reference

Wrapper class for the DDACE design of experiments library.

`#include <DACEIterator.H>`

Inheritance diagram for DACEIterator::



Public Methods

- DACEIterator (DakotaModel &model)
  primary constructor for building a standard iterator.
- DACEIterator (DakotaModel &model, int samples, int symbols, int seed, const DakotaString &sampling_method)
  alternate constructor for an iterator used for building approximations (inactive).
- ~DACEIterator ()
  destructor.
- void run_iterator ()
  run the iterator.
- const DakotaVariables & iterator_variable_results () const
  return the final iterator solution (variables).
- const DakotaResponse & iterator_response_results () const
  return the final iterator solution (response).
- void print_iterator_results (ostream &s) const
  print the final iterator results.
- void sampling_reset (int min_samples, short all_data_flag, short stats_flag)
  reset sampling iterator.
- const DakotaString & sampling_scheme () const
  return sampling name.
- void update_best (const DakotaRealVector &vars, const DakotaResponse &response, const int eval_num)
  compares current evaluation to best evaluation and updates best.

Private Methods

- void resolve_samples_symbols ()

  convenience function for resolving number of samples and number of symbols from input.

Private Attributes

- DakotaString daceMethod

  oas, lhs, oa_lhs, random, box_behnken_design, central_composite_design, or grid.

- int numSamples

  number of samples to be evaluated.

- int numSymbols

  number of symbols to be used in generating the sample set (inversely related to number of replications).

- int randomSeed

  seed for the random number generator (allows repeatability of results).

- short allDataFlag

  flag which triggers the update of allVars/allResponses for use by DakotaIterator::all_variables() and DakotaIterator::all_responses().

- DakotaVariables bestVariables

  best variables found during the study.

- DakotaResponse bestResponses

  best responses found during the study.

- Real bestObjectiveFn

  best objective function found during the study.

- Real bestViolations

  best constraint violations found during the study. In the current approach, constraint violation reduction takes strict precedence over objective function reduction.

- size_t numObjectiveFunctions

  number of objective functions. Used in update_best.

- size_t numNonlinearIneqConstraints

  number of nonlinear inequality constraints. Used in update_best.

- size_t numNonlinearEqConstraints

  number of nonlinear equality constraints. Used in update_best.

- DakotaRealVector multiObjWeights

  vector of multiobjective weights. Used in update_best.

- DakotaRealVector nonlinearIneqLowerBnds

vector of nonlinear inequality constraint lower bounds. Used in update_best.

- DakotaRealVector nonlinearIneqUpperBnds

  vector of nonlinear inequality constraint upper bounds. Used in update_best.

- DakotaRealVector nonlinearEqTargets

  vector of nonlinear equality constraint targets. Used in update_best.

6.16.1 Detailed Description

Wrapper class for the DDACE design of experiments library.

The DACEIterator 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 DakotaModel. It returns all generated samples and their corresponding responses as well as the best sample found.

6.16.2 Constructor & Destructor Documentation

6.16.2.1 DACEIterator::DACEIterator (DakotaModel & *model*)

primary constructor for building a standard iterator.

This constructor is called for a standard iterator built with data from probDescDB.

6.16.2.2 DACEIterator::DACEIterator (DakotaModel & *model*, int *samples*, int *symbols*, int *seed*, const DakotaString & *sampling_method*)

alternate constructor for an iterator used for building approximations (inactive).

This constructor is currently inactive, since the old DACEIterator instantiations within ApproximationInterface have been replaced with more general facilities within LayeredModel.

6.16.3 Member Function Documentation

6.16.3.1 void DACEIterator::run_iterator () `[virtual]`

run the iterator.

This function is the primary run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from DakotaIterator.

6.16.3.2 void DACEIterator::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.

The documentation for this class was generated from the following files:

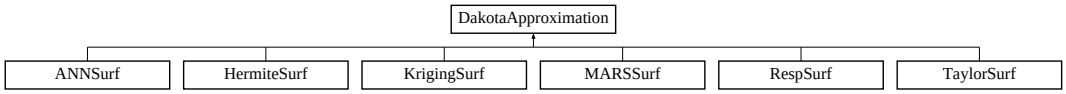
- DACEIterator.H
- DACEIterator.C

6.17 DakotaApproximation Class Reference

Base class for the approximation class hierarchy.

`#include <DakotaApproximation.H>`

Inheritance diagram for DakotaApproximation::



Public Methods

- DakotaApproximation ()

  default constructor.

- DakotaApproximation (const DakotaString &approx_type, const ProblemDescDB &problem_db)

  standard constructor for envelope.

- DakotaApproximation (const DakotaApproximation &approx)

  copy constructor.

- virtual ~DakotaApproximation ()

  destructor.

- DakotaApproximation operator= (const DakotaApproximation &approx)

  assignment operator.

- virtual void find_coefficients ()

  calculate the data fit coefficients using the currentPoints list of SurrogateDataPoints.

- virtual Real get_value (const DakotaRealVector &x)

  retrieve the approximate function value for a given parameter vector.

- virtual const DakotaRealVector & get_gradient (const DakotaRealVector &x)

  retrieve the approximate function gradient for a given parameter vector.

- virtual int required_samples (int num_vars)

  return the minimum number of samples required to build the derived class approximation type in num_vars dimensions.

- void build (int nv, int ns, const DakotaRealVectorArray &vars_samples, const DakotaRealVector &fn_samples, const DakotaRealVectorArray &grad_samples)

  build the surface from scratch. Populates currentPoints and invokes find_coefficients().

- void add_point_rebuild (const DakotaRealVector &x, const Real &f, const DakotaRealVector &grad_f)

  add a new point to the approximation and rebuild it.

- void set_bounds (const DakotaRealVector &lower, const DakotaRealVector &upper)

  set approximation lower and upper bounds (currently only used by graphics).

- void draw_surface ()

  render the approximate surface using the 3D graphics (2 variable problems only).

- const int & num_variables () const

  return the number of variables used in the approximation.

Protected Methods

- DakotaApproximation (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).

Protected Attributes

- int numVars

  number of variables in the approximation.

- int numCurrentPoints

  number of points in the currentPoints list.

- int numSamples

  number of samples passed to build() to construct the approximation.

- short gradientFlag

  flag signaling the use of gradient data in global approximation builds as indicated by the user's `use_gradients` *specification.*

- DakotaRealVector gradVector

  gradient of the approximation with respect to the variables.

- DakotaList< SurrogateDataPoint > currentPoints

  list of samples used to build the approximation.

- DakotaString approxType

  approximation type (long form for diagnostic I/O).

Private Methods

- DakotaApproximation * get_approx (const DakotaString &approx_type, const ProblemDescDB &problem_db)

  Used only by the envelope constructor to initialize approxRep to the appropriate derived type.

- void add_point (const DakotaRealVector &x, const Real &f, const DakotaRealVector &grad_f)

  add a new point to the approximation (used by build & add_point_rebuild).

Private Attributes

- DakotaRealVector approxLowerBounds

  approximation lower bounds (used only by 3D graphics).

- DakotaRealVector approxUpperBounds

  approximation upper bounds (used only by 3D graphics).

- DakotaApproximation * approxRep

  pointer to the letter (initialized only for the envelope).

- int referenceCount

  number of objects sharing approxRep.

6.17.1 Detailed Description

Base class for the approximation class hierarchy.

The DakotaApproximation class is the base class for the data fit surrogate class hierarchy in DAKOTA. One instance of a DakotaApproximation must be created for each function to be approximated (a vector of DakotaApproximations 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 (DakotaApproximation) serves as the envelope and one of the derived classes (selected in DakotaApproximation::get_approximation()) serves as the letter.

6.17.2 Constructor & Destructor Documentation

6.17.2.1 DakotaApproximation::DakotaApproximation ()

default constructor.

The default constructor is used in List<DakotaApproximation> instantiations. approxRep is NULL in this case (problem_db is needed to build a meaningful DakotaModel object). This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

6.17.2.2 DakotaApproximation::DakotaApproximation (const DakotaString & *approx_type*, const ProblemDescDB & *problem_db*)

standard constructor for envelope.

Envelope constructor only needs to extract enough data to properly execute get_approx, since DakotaApproximation(BaseConstructor, problem_db) builds the actual base class data for the derived approximations.

6.17.2.3 DakotaApproximation::DakotaApproximation (const DakotaApproximation & *approx*)

copy constructor.

Copy constructor manages sharing of approxRep and incrementing of referenceCount.

6.17.2.4 DakotaApproximation::~DakotaApproximation () [virtual]

destructor.

Destructor decrements referenceCount and only deletes approxRep when referenceCount reaches zero.

6.17.2.5 DakotaApproximation::DakotaApproximation (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 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 (an uninitialized pointer causes problems in ~DakotaApproximation).

6.17.3 Member Function Documentation

6.17.3.1 DakotaApproximation DakotaApproximation::operator= (const DakotaApproximation & *approx*)

assignment operator.

Assignment operator decrements referenceCount for old approxRep, assigns new approxRep, and increments referenceCount for new approxRep.

6.17.3.2 DakotaApproximation * DakotaApproximation::get_approx (const DakotaString & *approx_type*, const ProblemDescDB & *problem_db*) [private]

Used only by the envelope constructor to initialize approxRep to the appropriate derived type.

Used only by the envelope constructor to initialize approxRep to the appropriate derived type, as given by the approx_type parameter.

The documentation for this class was generated from the following files:

- DakotaApproximation.H
- DakotaApproximation.C

6.18 DakotaArray Class Template Reference

Template class for the Dakota bookkeeping array.

`#include <DakotaArray.H>`

Public Methods

- DakotaArray ()
  Default constructor.
- DakotaArray (size_t size)
  Constructor which takes an initial size.
- DakotaArray (size_t size, const T &initial_val)
  Constructor which takes an initial size and an initial value.
- DakotaArray (const DakotaArray< T > &a)
  Copy constructor.
- DakotaArray (const T *p, size_t size)
  Constructor, creates array of size, with initial value <T> p.
- ~DakotaArray ()
  Destructor.
- T & operator[ ] (ptrdiff_t i)
  Index operator, returns the ith value of the array.
- T & operator[ ] (size_t i)
  Index operator, returns the ith value of the array.
- const T & operator[ ] (ptrdiff_t i) const
  Index operator const, returns the ith value of the array.
- const T & operator[ ] (size_t i) const
  Index operator const, returns the ith value of the array.
- T & operator() (ptrdiff_t i)
  Index operator, not bounds checked.
- T & operator() (size_t i)
  Index operator, not bounds checked.
- const T & operator() (ptrdiff_t i) const
  Index operator const, not bounds checked.

- const T & operator() (size_t i) const

  Index operator const, not bounds checked.

- size_t length () const

  Returns size of array.

- void reshape (size_t sz)

  Resizes array to size sz.

- const T * data () const

  Returns pointer T to continuous data.*

- void testClass ()

  Class unit test method.

- DakotaArray< T > & operator= (const DakotaArray< T > &a)

  Normal const assignment operator.

- DakotaArray< T > & operator= (DakotaArray< T > &a)

  Normal assignment operator.

- DakotaArray< T > & operator= (const T &ival)

  Sets all elements in self to the value ival.

- operator T * () const

  Converts the {DakotaArray} to a standard C-style array. Use with care!

Private Methods

- void copy_array (const T *p, size_t size)

  Deep copies the array pointed to by {p} into this array.

6.18.1 Detailed Description

template<class T> class DakotaArray< T >

Template class for the Dakota bookkeeping array.

An array class template that provides additional functionality that is specific to Dakota's needs. The DakotaArray class adds additional functionallity needed by Dakota to the inherited base array class. The DakotaArray class can inherite from either the STL or RW vector classes.

6.18.2 Constructor & Destructor Documentation

6.18.2.1 template<class T> DakotaArray< T >::DakotaArray (const T * *p*, size_t *size*)

Constructor, creates array of size, with initial value <T> p.

Assigns up to size values in array to p. Calls the private method copy_array

6.18.3 Member Function Documentation

6.18.3.1 template<class T> const T * DakotaArray< T >::data () const

Returns pointer T* to continuous data.

Returns a c style pointer to the data within the array. USE WITH CARE. Needed to mimick RW vector class, is used in the operator(). Uses the STL front method.

6.18.3.2 template<class T> void DakotaArray< T >::testClass ()

Class unit test method.

Unit test method for the DakotaArray class. Provides a quick way to test the basic functionallity of the class. Utilizes the assert function to test for correctness, will fail if an unexpected answer is received.

6.18.3.3 template<class T> DakotaArray< T > & DakotaArray< T >::operator= (const T & *ival*)

Sets all elements in self to the value ival.

Assigns all values of array to the value passed in as ival. For the Rogue Wave case utilizes base class operator=(ival),i while for the ANSI case uses the STL assign() method.

6.18.3.4 template<class T> DakotaArray< T >::operator T * () const

Converts the {DakotaArray} to a standard C-style array. Use with care!

The operator() returns a c style pointer to the data within the array. Calls the data() method. USE WITH CARE.

6.18.3.5 template<class T> void DakotaArray< T >::copy_array (const T * *p*, size_t *size*) [private]

Deep copies the array pointed to by {p} into this array.

Copy an array of type T into the DakotaArray Private function for {operator=(const T *p)} and the constructor {DakotaArray(const T* p, size_t size)}.

The documentation for this class was generated from the following file:

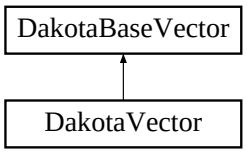
- DakotaArray.H

6.19 DakotaBaseVector Class Template Reference

Base class for the DakotaMatrix and DakotaVector classes.

`#include <DakotaBaseVector.H>`

Inheritance diagram for DakotaBaseVector::



Public Methods

- DakotaBaseVector ()
  Default constructor.
- DakotaBaseVector (size_t size)
  Constructor, creates vector of size.
- DakotaBaseVector (size_t size, const T &initial_val)
  Constructor, creates vector of size with initial value of initial_val.
- ~DakotaBaseVector ()
  Destructor.
- DakotaBaseVector (const DakotaBaseVector< T > &a)
  Default copy constructor.
- DakotaBaseVector (const T *p, size_t size)
  Alternate copy constructor.
- DakotaBaseVector< T > & operator= (const DakotaBaseVector< T > &a)
  Normal assignment operator.
- DakotaBaseVector< T > & operator= (const T &ival)
  Assigns all values of vector to ival.
- T & operator[ ] (ptrdiff_t i)
  Returns the object at index i, (can use as lvalue).
- T & operator[ ] (size_t i)
  Returns the object at index i, (can use as lvalue).
- const T & operator[ ] (ptrdiff_t i) const

Returns the object at index i, const (can't use as lvalue).

- const T & operator[ ] (size_t i) const
  Returns the object at index i, const (can't use as lvalue).
- T & operator() (ptrdiff_t i)
  Index operator, not bounds checked.
- T & operator() (size_t i)
  Index operator, not bounds checked.
- const T & operator() (ptrdiff_t i) const
  Index operator const , not bounds checked.
- const T & operator() (size_t i) const
  Index operator const , not bounds checked.
- size_t length () const
  Returns size of vector.
- void reshape (size_t sz)
  Resizes vector to size sz.
- const T * data () const
  Returns pointer to standard C array use with care.

Protected Attributes

- T * array_
  Protected data member to hold pointer to front of vector.
- size_t npts_
  Protected data member which holds number of points in array.

6.19.1 Detailed Description

template<class T> class DakotaBaseVector< T >

Base class for the DakotaMatrix and DakotaVector classes.

The DakotaBaseVector class is the base class for the DakotaMatrix class. It is used to define a common vector interface for both the STL and RW vector classes. If the STL version is based on the valarray class then some basic vector operations such as + , * are available

6.19.2 Constructor & Destructor Documentation

6.19.2.1 template<class T> DakotaBaseVector< T >::DakotaBaseVector (size_t *size*, const T & *initial_val*)

Constructor, creates vector of size with initial value of initial_val.

Constructor which takes an initial size and an initial value, allocates an area of initial size and initializes it with input value. Calls base class constructor

6.19.3 Member Function Documentation

6.19.3.1 template<class T> void DakotaBaseVector< T >::reshape (size_t *sz*)

Resizes vector to size sz.

Resizes the array to size sz by calling the STL resize method, and sets the private data member npts_equal to sz. Needed to mimick the RW vector class

6.19.3.2 template<class T> const T * DakotaBaseVector< T >::data () const

Returns pointer to standard C array use with care.

Returns a c style pointer to the data within the array. USE WITH CARE. Needed to mimick RW vector class.

The documentation for this class was generated from the following file:

- DakotaBaseVector.H

6.20 DakotaBiStream Class Reference

The binary input stream class. Overloads the >> operator for all data types.

`#include <DakotaBinStream.H>`

Public Methods

- DakotaBiStream ()
  Default constructor, need to open.
- DakotaBiStream (const char *s)
  Constructor takes name of input file.
- DakotaBiStream (const char *s, int flags)
  Constructor takes name of input file, flags.
- ~DakotaBiStream ()
  Destructor, calls xdr_destroy to delete xdr stream.
- DakotaBiStream & operator>> (DakotaString &)
  Binary Input stream operator>>.
- DakotaBiStream & operator>> (char *)
  Input operator, reads char from binary stream DakotaBiStream.*
- DakotaBiStream & operator>> (char &)
  Input operator, reads char from binary stream DakotaBiStream.
- DakotaBiStream & operator>> (int &)
  Input operator, reads int from binary stream DakotaBiStream.*
- DakotaBiStream & operator>> (long &)
  Input operator, reads long from binary stream DakotaBiStream.
- DakotaBiStream & operator>> (short &)
  Input operator, reads short from binary stream DakotaBiStream.
- DakotaBiStream & operator>> (double &)
  Input operator, reads double from binary stream DakotaBiStream.
- DakotaBiStream & operator>> (float &)
  Input operator, reads float from binary stream DakotaBiStream.
- DakotaBiStream & operator>> (unsigned char &)
  Input operator, reads unsigned char from binary stream DakotaBiStream.*

- DakotaBiStream & operator>> (unsigned int &)

  Input operator, reads unsigned int from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (unsigned long &)

  Input operator, reads unsigned long from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (unsigned short &)

  Input operator, reads unsigned short from binary stream DakotaBiStream.

Private Attributes

- XDR xdrInBuf

  XDR input stream buffer.

- char inBuf [256]

  Buffer to hold data as it is read in.

6.20.1 Detailed Description

The binary input stream class. Overloads the >> operator for all data types.

The DakotaBiStream class is a binary input class which overloads the >> operator for all standard data types(int, char, float, etc). The class relies on the methods within the ifstream base class. The DakotaBiStream class inherits from the ifstream class. The class also utilize rpc/xdr to construct machine independent binary files. The Dakota restart files can now be moved from host to host. These motivation to develop these classes was to replace the Rogue wave classes which Dakota historically used for binary I/O.

6.20.2 Constructor & Destructor Documentation

6.20.2.1 DakotaBiStream::DakotaBiStream ()

Default constructor, need to open.

Default constructor, allocates xdr stream , but does not call the open method. The open method must be called before stream can be read.

6.20.2.2 DakotaBiStream::DakotaBiStream (const char * *s*)

Constructor takes name of input file.

Constructor which takes a char* filename. Calls the base class open method with the filename and no other arguments. Also allocates the xdr stream.

6.20.2.3 DakotaBiStream::DakotaBiStream (const char * *s*, int *flags*)

Constructor takes name of input file, flags.

Constructor which takes a char* filename and int flags. Calls the base class open method with the filename and flags as arguments. Also allocates xdr stream.

6.20.2.4 DakotaBiStream::~DakotaBiStream ()

Destructor, calls xdr_destroy to delete xdr stream.

Destructor, destroys the xdr stream allocated in constructor

6.20.3 Member Function Documentation

6.20.3.1 DakotaBiStream & DakotaBiStream::operator>> (DakotaString & *ds*)

Binary Input stream operator>>.

The DakotaString input operator must first read both the xdr buffer size and the size of the string written. Once these our read it can then read and convert the DakoaString correctly.

6.20.3.2 DakotaBiStream & DakotaBiStream::operator>> (char * *s*)

Input operator, reads char* from binary stream DakotaBiStream.

Reading char array is a special case. The method has no way of knowing if the length to the input array is large enough, it assumes it is one char longer than actual string, (Null terminator added). As with the DakotaString the size of the xdr buffer as well as the char array size written must be read from the stream prior to reading and converting the char array.

The documentation for this class was generated from the following files:

- DakotaBinStream.H
- DakotaBinStream.C

6.21 DakotaBoStream Class Reference

The binary output stream class. Overloads the << operator for all data types.

`#include <DakotaBinStream.H>`

Public Methods

- DakotaBoStream ()
  Default constructor, need to open.
- DakotaBoStream (const char *s)
  Constructor takes name of input file.
- DakotaBoStream (const char *s, int flags)
  Constructor takes name of input file, flags.
- ~DakotaBoStream ()
  Destructor, calls xdr_destroy to delete xdr stream.
- void testClass ()
  Performs unit testing for the DakotaBoStream class.
- DakotaBoStream & operator<< (const DakotaString &)
  Binary Output stream operator<<.
- DakotaBoStream & operator<< (const char *)
  Output operator, writes char TO binary stream DakotaBoStream.*
- DakotaBoStream & operator<< (const char &c)
  Output operator, writes char to binary stream DakotaBoStream.
- DakotaBoStream & operator<< (const int &i)
  Output operator, writes int to binary stream DakotaBoStream.
- DakotaBoStream & operator<< (const long &l)
  Output operator, writes long to binary stream DakotaBoStream.
- DakotaBoStream & operator<< (const double &d)
  Output operator, writes double to binary stream DakotaBoStream.
- DakotaBoStream & operator<< (const short &s)
  Output operator, writes short to binary stream DakotaBoStream.
- DakotaBoStream & operator<< (const float &f)
  Output operator, writes float to binary stream DakotaBoStream.

- DakotaBoStream & operator<< (const unsigned char &c)
  Output operator, writes unsigned char to binary stream DakotaBoStream.
- DakotaBoStream & operator<< (const unsigned int &i)
  Output operator, writes unsigned int to binary stream DakotaBoStream.
- DakotaBoStream & operator<< (const unsigned long &l)
  Output operator, writes unsigned long to binary stream DakotaBoStream.
- DakotaBoStream & operator<< (const unsigned short &s)
  Output operator, writes unsigned short to binary stream DakotaBoStream.

Private Attributes

- XDR xdrOutBuf
  XDR output stream buffer.
- char outBuf [256]
  Buffer to hold converted data before it is written.

6.21.1 Detailed Description

The binary output stream class. Overloads the << operator for all data types.

The DakotaBoStream class is a binary output classes which overloads the << operator for all standard data types (int, char, float, etc). The class relies on the built in write methods within the ostream base classes. DakotaBoStream inherits from the ofstream class. The motivation to develop this class was to replace the Rogue wave class which Dakota historically used for binary I/O. The class also utilize rpc/xdr to construct machine independent binary files. The Dakota restart files can now be moved between hosts. These motivation to develop these classes was to replace the RW classes which Dakota historically used for binary I/O.

6.21.2 Constructor & Destructor Documentation

6.21.2.1 DakotaBoStream::DakotaBoStream ()

Default constructor, need to open.

Default constructor, allocates xdr stream , but does not call the open() method. The open() method must be called before stream can be written to.

6.21.2.2 DakotaBoStream::DakotaBoStream (const char * s)

Constructor takes name of input file.

Constructor, takes char * filename as argument. Calls base class open method with filename and no other arguments. Also allocates xdr stream

6.21.2.3 DakotaBoStream::DakotaBoStream (const char * *s*, int *flags*)

Constructor takes name of input file, flags.

Constructor, takes char * filename and int flagss as arguments. Calls base class open method with filename and flags as arguments. Also allocates xdr stream

6.21.3 Member Function Documentation

6.21.3.1 void DakotaBoStream::testClass ()

Performs unit testing for the DakotaBoStream class.

Unit test method for the DakotaBinStream class. Provides a quick way to test the basic functionallity of the class. Utilizes the assert function to test for corretness, will fail if an expected answer is not received.

6.21.3.2 DakotaBoStream & DakotaBoStream::operator<< (const DakotaString & *ds*)

Binary Output stream operator<<.

The DakotaString operator<< must first write the xdr buffer size and the original string size to the stream. The input operator needs this information to be able to correctly read and convert the DakotaString.

6.21.3.3 DakotaBoStream & DakotaBoStream::operator<< (const char * *s*)

Output operator, writes char* TO binary stream DakotaBoStream.

The output of char* is the same as the output of the DakotaString. The size of the xdr buffer and the size of the string must be written first, then the string itself.

The documentation for this class was generated from the following files:

- DakotaBinStream.H
- DakotaBinStream.C

6.22 DakotaGraphics Class Reference

The DakotaGraphics class provides a single interface to 2D (motif) and 3D (PLPLOT) graphics as well as tabular cataloguing of data for post-processing with Matlab, Tecplot, etc.

`#include <DakotaGraphics.H>`

Public Methods

- DakotaGraphics ()
  constructor.
- ~DakotaGraphics ()
  destructor.
- void create_plots_2d (const DakotaVariables &vars, const DakotaResponse &response)
  creates the 2d graphics window and initializes the plots.
- void create_tabular_datastream (const DakotaVariables &vars, const DakotaResponse &response, const DakotaString &tabular_data_file)
  opens the tabular data file stream and prints the headings.
- void add_datapoint (const DakotaVariables &vars, const DakotaResponse &response)
  adds data to the 2d graphics and tabular data file.
- void show_data_3d (DakotaRealArray &X, DakotaRealArray &Y, DakotaRealMatrix &F)
  generate a new 3d plot for F(X,Y).

Private Attributes

- Graphics2D * graphics2D
  pointer to the 2D graphics object.
- short win2dOn
  flag to indicate if 2D graphics window is active.
- short win3dOn
  flag to indicate if 3D graphics window is active.
- int graphicsCntr
  used for x axis values in 2D graphics and for 1st column in tabular data.
- short tabularDataFlag
  flag to indicate if tabular data stream is active.
- ofstream tabularDataFStream

file stream for tabulation of graphics data within compute_response.

6.22.1 Detailed Description

The DakotaGraphics class provides a single interface to 2D (motif) and 3D (PLPLOT) graphics as well as tabular cataloguing of data for post-processing with Matlab, Tecplot, etc.

There is only one DakotaGraphics object (dakotaGraphics) and it is global (for convenient access from strategies, models, and approximations).

6.22.2 Member Function Documentation

6.22.2.1 void DakotaGraphics::create_plots_2d (const DakotaVariables & *vars*, const DakotaResponse & *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).

The documentation for this class was generated from the following files:

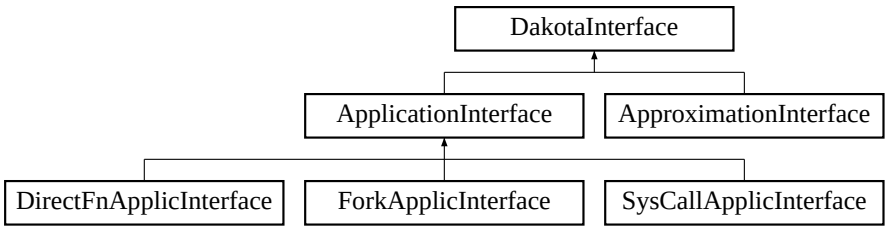
- DakotaGraphics.H
- DakotaGraphics.C

6.23 DakotaInterface Class Reference

Base class for the interface class hierarchy.

`#include <DakotaInterface.H>`

Inheritance diagram for DakotaInterface::



Public Methods

- DakotaInterface ()
  default constructor.
- DakotaInterface (ProblemDescDB &problem_db, const size_t &num_acv, const size_t &num_fns)
  standard constructor for envelope.
- DakotaInterface (const DakotaInterface &interface)
  copy constructor.
- virtual ~DakotaInterface ()
  destructor.
- DakotaInterface operator= (const DakotaInterface &interface)
  assignment operator.
- virtual void map (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response, const int asynch_flag=0)
  the function evaluator: provides a "mapping" from the variables to the responses.
- virtual const DakotaArray< DakotaResponse > & synch ()
  recovers data from a series of asynchronous evaluations (blocking).
- virtual const DakotaList< DakotaResponse > & synch_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 DakotaIntArray &message_lengths, const int &max_iterator_concurrency)

  allocate communicator partitions for concurrent evaluations within an iterator and concurrent multiprocessor analyses within an evaluation.

- virtual void free_communicators ()

  deallocate communicator partitions for concurrent evaluations within an iterator and concurrent multiprocessor analyses within an evaluation.

- virtual int asynch_local_evaluation_concurrency () const

  return the user-specified concurrency for asynch local evaluations.

- virtual DakotaString interface_synchronization () const

  return the user-specified interface synchronization.

- virtual int minimum_samples () const

  returns the minimum number of samples required to build a particular ApproximationInterface (used by SurrLayeredModels).

- virtual void build_global_approximation (DakotaIterator &dace_iterator)

  builds a global approximation for use as a surrogate.

- virtual void build_local_approximation (DakotaModel &actual_model)

  builds a local approximation for use as a surrogate.

- virtual void update_approximation (const DakotaRealVector &x_star, const DakotaResponse &response_star)

  updates an existing global approximation with new data.

- const DakotaIntList & synch_nowait_completions ()

  returns id's matching response list from synch_nowait().

- const DakotaString & interface_type () const

  returns the interface type.

- int total_eval_counter () const

  returns the total number of evaluations of the interface.

- int new_eval_counter () const

  returns the number of new (nonduplicate) evaluations of the interface.

- short multi_proc_eval_flag () const

  returns a flag signaling the use of multiprocessor evaluation partitions.

- short iterator_dedicated_master_flag () const

  returns a flag signaling the use of a dedicated master processor for iterator scheduling.

Protected Methods

- DakotaInterface (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).

Protected Attributes

- DakotaString interfaceType

  interface type may be (1) application: system, fork, direct, or xml; or (2) approximation: ann, rsm, mars, hermite, ksm, mpa, taylor, or hierarchical.

- int fnEvalId

  total evaluation counter.

- int newFnEvalId

  new (non-duplicate) evaluation counter.

- DakotaIntList beforeSynchIdList

  bookkeeps fnEvalId's of _all_ asynchronous evaluations (new & duplicate).

- DakotaArray< DakotaResponse > rawResponseArray

  The complete array of responses returned after a blocking schedule of asynchronous evaluations.

- DakotaList< DakotaResponse > rawResponseList

  The partial list of responses returned after a nonblocking schedule of asynchronous evaluations.

- DakotaIntList completionList

  identifies the responses in rawResponseList for nonblocking schedules.

- short multiProcEvalFlag

  flag for multiprocessor evaluation partitions (evalComm).

- short iteratorDedMasterFlag

  flag for dedicated master partitioning at the iterator level.

- short verboseFlag

  flag for verbose interface output.

- short debugFlag

  flag for really verbose (debug) interface output.

Private Methods

- DakotaInterface * get_interface (ProblemDescDB &problem_db, const size_t &num_acv, const size_t &num_fns)

  Used by the envelope to instantiate the correct letter class.

Private Attributes

- DakotaInterface * interfaceRep

  pointer to the letter (initialized only for the envelope).

- int referenceCount

  number of objects sharing interfaceRep.

6.23.1 Detailed Description

Base class for the interface class hierarchy.

The DakotaInterface class hierarchy provides the part of a DakotaModel that is responsible for mapping a set of DakotaVariables into a set of DakotaResponses. 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 (DakotaInterface) serves as the envelope and one of the derived classes (selected in DakotaInterface::get_interface()) serves as the letter.

6.23.2 Constructor & Destructor Documentation

6.23.2.1 DakotaInterface::DakotaInterface ()

default constructor.

used in DakotaModel envelope class instantiations

6.23.2.2 DakotaInterface::DakotaInterface (ProblemDescDB & *problem_db*, const size_t & *num_acv*, const size_t & *num_fns*)

standard constructor for envelope.

Used in DakotaModel instantiation to build the envelope. This constructor only needs to extract enough data to properly execute get_interface, since DakotaInterface::DakotaInterface(BaseConstructor, problem_db) builds the actual base class data inherited by the derived interfaces.

6.23.2.3 DakotaInterface::DakotaInterface (const DakotaInterface & *interface*)

copy constructor.

Copy constructor manages sharing of interfaceRep and incrementing of referenceCount.

6.23.2.4 DakotaInterface::~DakotaInterface () [virtual]

destructor.

Destructor decrements referenceCount and only deletes interfaceRep if referenceCount is zero.

6.23.2.5 DakotaInterface::DakotaInterface (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 (an uninitialized pointer causes problems in ~DakotaInterface).

6.23.3 Member Function Documentation

6.23.3.1 DakotaInterface DakotaInterface::operator= (const DakotaInterface & *interface*)

assignment operator.

Assignment operator decrements referenceCount for old interfaceRep, assigns new interfaceRep, and increments referenceCount for new interfaceRep.

6.23.3.2 DakotaInterface * DakotaInterface::get_interface (ProblemDescDB & *problem_db*, const size_t & *num_acv*, const size_t & *num_fns*) [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, as given by the interfaceType attribute.

6.23.4 Member Data Documentation

6.23.4.1 DakotaArray<DakotaResponse> DakotaInterface::rawResponseArray [protected]

The complete array of responses returned after a blocking schedule of asynchronous evaluations.

The array is the raw set of responses corresponding to all asynchronous map calls. This raw array is postprocessed (i.e., finite difference gradients merged) in DakotaModel::synchronize() where it becomes responseArray.

6.23.4.2 DakotaList<DakotaResponse> DakotaInterface::rawResponseList [protected]

The partial list of responses returned after a nonblocking schedule of asynchronous evaluations.

The list is a partial set of completions which must be identified through the use of completionList. Postprocessing from raw to combined form (i.e., finite difference gradient merging) is not currently supported in DakotaModel::synchronize_nowait().

The documentation for this class was generated from the following files:

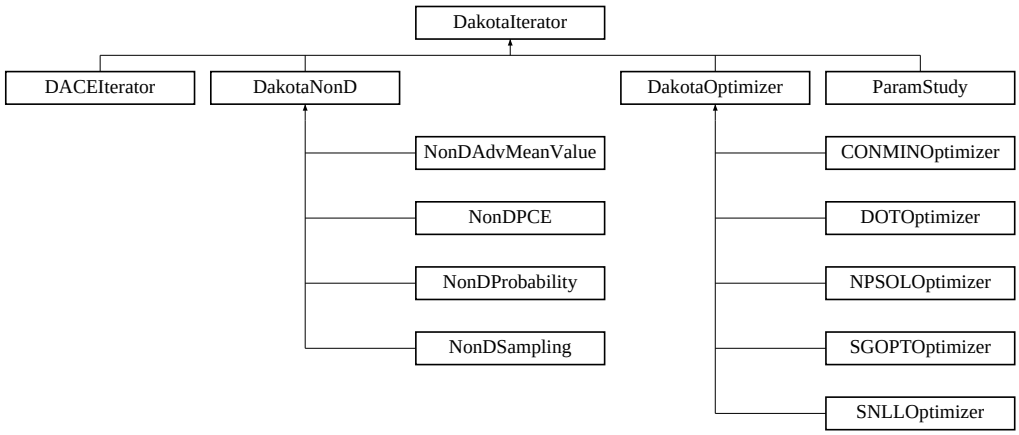
- DakotaInterface.H
- DakotaInterface.C

6.24 DakotaIterator Class Reference

Base class for the iterator class hierarchy.

`#include <DakotaIterator.H>`

Inheritance diagram for DakotaIterator::



Public Methods

- DakotaIterator ()
  default constructor.
- DakotaIterator (DakotaModel &model)
  standard constructor for envelope.
- DakotaIterator (const DakotaIterator &iterator)
  copy constructor.
- virtual ~DakotaIterator ()
  destructor.
- DakotaIterator operator= (const DakotaIterator &iterator)
  assignment operator.
- virtual void run_iterator ()
  run the iterator.
- virtual const DakotaVariables & iterator_variable_results () const
  return the final iterator solution (variables).
- virtual const DakotaResponse & iterator_response_results () const
  return the final iterator solution (response).

- virtual void print_iterator_results (ostream &s) const

  print the final iterator results.

- virtual void multi_objective_weights (const DakotaRealVector &multi_obj_wts)

  set the relative weightings for multiple objective functions. Used by ConcurrentStrategy for Pareto set optimization.

- virtual void sampling_reset (int min_samples, short all_data_flag, short stats_flag)

  reset sampling iterator.

- virtual const DakotaString & sampling_scheme () const

  return sampling name.

- void user_defined_model (const DakotaModel &the_model)

  set the model.

- DakotaModel & user_defined_model () const

  return the model.

- const DakotaString & method_name () const

  return the method name.

- int maximum_concurrency () const

  return the maximum concurrency supported by the iterator.

- const DakotaRealVectorArray & all_variables () const

  return the complete set of evaluated variables (used by ApproximationInterface::build_approximation).

- const DakotaArray< DakotaResponse > & all_responses () const

  return the complete set of computed responses (used by ApproximationInterface::build_approximation).

- short is_null () const

  function to check iteratorRep (does this envelope contain a letter).

Protected Methods

- DakotaIterator (BaseConstructor, DakotaModel &model)

  constructor initializes the base class part of letter classes (BaseConstructor overloading avoids infinite recursion in the derived class constructors - Coplien, p. 139).

- DakotaIterator (NoDBBaseConstructor, DakotaModel &model)

  base class for iterator classes constructed on the fly (no DB queries).

Protected Attributes

- DakotaModel & userDefinedModel

  class member reference for the model passed into the constructor.

- const ProblemDescDB & probDescDB

  class member reference to the problem description database.

- DakotaString methodName

  name of the iterator (the user's method spec).

- int maxIterations

  maximum number of iterations for the iterator.

- int maxFunctionEvals

  maximum number of fn evaluations for the iterator.

- int numFunctions

  number of response functions.

- int maxConcurrency

  maximum coarse-grained concurrency.

- int numContinuousVars

  number of active continuous vars.

- int numDiscreteVars

  number of active discrete vars.

- int numVars

  total number of vars. (active and inactive).

- DakotaIntArray activeSetVector

  this vector tracks the data requirements for the response functions. It uses a 0 value for inactive functions and, for active functions, sums 1 for value, 2 for gradient, and 4 for Hessian.

- DakotaString gradientType

  type of gradient data: "analytic", "numerical", "mixed", or "none".

- DakotaString hessianType

  type of Hessian data: "analytic" or "none".

- DakotaString finiteDiffType

  type of finite difference interval: "central" or "forward".

- DakotaString methodSource

  source of finite difference routine: "dakota" or "vendor".

- Real finiteDiffStepSize

  relative finite difference step size.

- DakotaIntList mixedGradAnalyticIds
  for mixed gradients, contains ids of functions with analytic gradients.
- DakotaIntList mixedGradNumericalIds
  for mixed gradients, contains ids of functions with numerical gradients.
- DakotaString outputLevel
  iterator verbosity: "verbose", "normal", "quiet", or "debug".
- short verboseOutput
  convenience flag for outputLevel == "verbose".
- short debugOutput
  convenience flag for outputLevel == "debug".
- short asynchFlag
  copy of the model's asynchronous evaluation flag.
- DakotaRealVectorArray allVariables
  array of all variables evaluated (used by ApproximationInterface).
- DakotaArray< DakotaResponse > allResponses
  array of all responses computed (used by ApproximationInterface).

Static Protected Attributes

- DakotaModel & staticModel = dummy_model
  static model reference used by OPT++, NPSOL, NonDAMV.

Private Methods

- DakotaIterator * get_iterator (DakotaModel &model)
  Used by the envelope to instantiate the correct letter class.
- void populate_gradient_vars ()
  Used only by constructor functions to define gradient variables for use within the iterator hierarchy.

Private Attributes

- DakotaIterator * iteratorRep
  pointer to the letter (initialized only for the envelope).
- int referenceCount
  number of objects sharing iteratorRep.

6.24.1 Detailed Description

Base class for the iterator class hierarchy.

The DakotaIterator 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 (DakotaIterator) serves as the envelope and one of the derived classes (selected in DakotaIterator::get_iterator()) serves as the letter.

6.24.2 Constructor & Destructor Documentation

6.24.2.1 DakotaIterator::DakotaIterator ()

default constructor.

The default constructor is used in Vector<DakotaIterator> instantiations and for initialization of DakotaIterator objects contained in DakotaStrategy derived classes (see derived class header files). iteratorRep is NULL in this case (a populated problem_db is needed to build a meaningful DakotaIterator object). This makes it necessary to check for NULL pointers in the copy constructor, assignment operator, and destructor.

6.24.2.2 DakotaIterator::DakotaIterator (DakotaModel & *model*)

standard constructor for envelope.

Used in iterator instantiations within strategy constructors. Envelope constructor only needs to extract enough data to properly execute get_iterator, since DakotaIterator(BaseConstructor, model) builds the actual base class data inherited by the derived iterators.

6.24.2.3 DakotaIterator::DakotaIterator (const DakotaIterator & *iterator*)

copy constructor.

Copy constructor manages sharing of iteratorRep and incrementing of referenceCount.

6.24.2.4 DakotaIterator::~DakotaIterator () [virtual]

destructor.

Destructor decrements referenceCount and only deletes iteratorRep when referenceCount reaches zero.

6.24.2.5 DakotaIterator::DakotaIterator (BaseConstructor, DakotaModel & *model*) [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. 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 (an uninitialized pointer causes problems in ~DakotaIterator).

6.24.2.6 DakotaIterator::DakotaIterator (NoDBBaseConstructor, DakotaModel & *model*) [protected]

base class for iterator classes constructed on the fly (no DB queries).

This constructor also builds base class data for inherited iterators. However, it is used for on-the-fly instantiations for which DB queries cannot be used (e.g., ApproximationInterface instantiation of DACEIterator or NonDProbability, AMV usage of optimizers, etc.). Therefore it only sets attributes taken from the incoming model.

6.24.3 Member Function Documentation

6.24.3.1 DakotaIterator DakotaIterator::operator= (const DakotaIterator & *iterator*)

assignment operator.

Assignment operator decrements referenceCount for old iteratorRep, assigns new iteratorRep, and increments referenceCount for new iteratorRep.

6.24.3.2 void DakotaIterator::run_iterator () [virtual]

run the iterator.

This function is the primary run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented in DACEIterator, DakotaNonD, DakotaOptimizer, and ParamStudy.

6.24.3.3 DakotaIterator * DakotaIterator::get_iterator (DakotaModel & *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 methodName attribute.

6.24.3.4 void DakotaIterator::populate_gradient_vars () [private]

Used only by constructor functions to define gradient variables for use within the iterator hierarchy.

Convenience function for constructors. Populates gradient and Hessian data attributes from the problem description database.

The documentation for this class was generated from the following files:

- DakotaIterator.H
- DakotaIterator.C

6.25 DakotaList Class Template Reference

Template class for the Dakota bookkeeping list.

`#include <DakotaList.H>`

Public Methods

- DakotaList ()
  Default constructor.
- DakotaList (const DakotaList< T > &a)
  Copy constructor.
- ~DakotaList ()
  Destructor.
- DakotaList< T > & operator= (const DakotaList< T > &)
  assignment operator.
- void testClass ()
  Class unit test method.
- size_t entries () const
  Returns the number of items that are currently in the list.
- void append (const T &a)
  Adds the item a to the end of the list.
- T get ()
  Returns the last item on the list and removes it.
- T removeAt (size_t index)
  Removes and returns the item at the specified index.
- int remove (const T &a)
  Removes the specified item from the list.
- void insert (const T &a)
  Adds the item a to the end of the list.
- int contains (const T &a) const
  Returns TRUE if list contains object a, returns FALSE otherwise.
- int find (int(*testFun)(const T &, void *), void *d, T &k) const
  Returns TRUE if the list contains an object which the user defined function finds.

- size_t index (int(*testFun)(const T &, void *), void *d) const

  Returns the index of object which the user defined test function finds.

- void sort (int(*sortFun)(const T &, const T &))

  Sorts the list into an order based on the predefined sort function.

- size_t index (const T &a) const

  Returns the index of the object.

- size_t occurrencesOf (const T &a) const

  Returns the number of items in the list equal to object.

- bool isEmpty ()

  Returns TRUE if list is empty, returns FALSE otherwise.

- T & operator[ ] (size_t i)

  Returns the object at index i (can use as lvalue).

- const T & operator[ ] (size_t i) const

  Returns the object at index i, const (can't use as lvalue).

6.25.1 Detailed Description

template<class T> class DakotaList< T >

Template class for the Dakota bookkeeping list.

The DakotaList is the common list class for Dakota. It inherits from either the RW list class or the STL list class. Extends the base list class to add Dakota specific methods Builds upon the previously existing DakotaValList class

6.25.2 Member Function Documentation

6.25.2.1 template<class T> void DakotaList< T >::testClass ()

Class unit test method.

Unit test method for the DakotaList class. Provides a quick way to test the basic functionallity of the class. Utilizes the assert function to test for correctness, will fail if an unexpected answer is received.

6.25.2.2 template<class T> void DakotaList< T >::append (const T & *a*)

Adds the item a to the end of the list.

Insert item at the end of list, calls STL push_back method which places the object at the end of the list. Same as the insert() method.

6.25.2.3 template<class T> T DakotaList< T >::get ()

Returns the last item on the list and removes it.

Remove and return item from front of list. Returns the object pointed to by the STL front iterator. It also deletes the first node by calling the STL erase method. The erase() method handles all aspects of removing a node from the list.

6.25.2.4 template<class T> T DakotaList< T >::removeAt (size_t *index*)

Removes and returns the item at the specified index.

Removes the item at the index specified. Uses a STL iterator to step to the appropriate position in the list, and then calls the STL erase() method(). The erase() method handles all aspects of removing a node from the list

6.25.2.5 template<class T> int DakotaList< T >::remove (const T & *a*)

Removes the specified item from the list.

Remove the item from the list, uses STL iterator to find the object. It then calls the STL erase() method which handles all the aspects of doing a remove.

6.25.2.6 template<class T> void DakotaList< T >::insert (const T & *a*)

Adds the item a to the end of the list.

Insert item at the end of list, calls STL push_back method which places the object at the end of the list. Same as the append() method.

6.25.2.7 template<class T> int DakotaList< T >::contains (const T & *a*) const

Returns TRUE if list contains object a, returns FALSE otherwise.

Uses a STL iterator to step through the list. Returns a true as soon as the specified object is found.

6.25.2.8 template<class T> int DakotaList< T >::find (int(* *testFun*)(const T &, void *), void * *d*, T & *k*) const

Returns TRUE if the list contains an object which the user defined function finds.

The find method mimicks the RW find algorithm by utilizing the FunctionCompare class and the STL find_if algorithm. The find_if method returns an iterator. The iterator is then compared against the iterator that is returned by the method end() to determine if object was found.

6.25.2.9 template<class T> size_t DakotaList< T >::index (int(* *testFun*)(const T &, void *), void * *d*) const

Returns the index of object which the user defined test function finds.

The index method mimicks the RW index algorithm by utilizing the FunctionCompare class and the STL find_if algorithm. The find_if method returns an iterator. The iterator is then used to find the position of the object.

6.25.2.10 template<class T> void DakotaList< T >::sort (int(* *sortFun*)(const T &, const T &))

Sorts the list into an order based on the predefined sort function.

The sort method utilizes the SortCompare class and the STL sort algorithm to sort a list based on the predefined function sortFun. Each type T should have a defined sort method if you wish to sort the specific data. Note: Not supported under SOLARIS!

6.25.2.11 template<class T> size_t DakotaList< T >::index (const T & *a*) const

Returns the index of the object.

Returns the index of the item in the list, uses STL iterator to step through the list. Returns the index of the first instance of the object, there may be more than one in the list.

6.25.2.12 template<class T> size_t DakotaList< T >::occurrencesOf (const T & *a*) const

Returns the number of items in the list equal to object.

Uses an STL iterator to step through the list and count the number of occurences of the specified object.

6.25.2.13]

template<class T> T & DakotaList< T >::operator[ ] (size_t *i*)

Returns the object at index i (can use as lvalue).

Return item at position i of list, steps through using STL iterator Once object is found it returns the value poiinted to by the iterator.

6.25.2.14]

template<class T> const T & DakotaList< T >::operator[ ] (size_t *i*) const

Returns the object at index i, const (can't use as lvalue).

Return const item at position i of list, steps through the list using an STL iterator. Once object is found it returns the value poiinted to by the iterator.

The documentation for this class was generated from the following file:

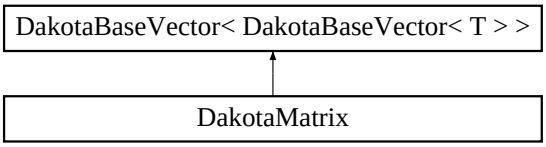
- DakotaList.H

6.26 DakotaMatrix Class Template Reference

Template class for the Dakota numerical matrix.

`#include <DakotaMatrix.H>`

Inheritance diagram for DakotaMatrix::



Public Methods

- DakotaMatrix (size_t num_rows=0, size_t num_cols=0)

  Constructor, takes number of rows, and number of columns as arguments.

- ~DakotaMatrix ()

  Destructor.

- DakotaMatrix< T > & operator= (const T &ival)

  Sets all elements in the matrix to ival.

- size_t num_rows () const

  Returns the number of rows for the matrix.

- size_t num_columns () const

  Returns the number of columns for the matrix.

- void reshape_2d (size_t num_rows, size_t num_cols)

  Resizes the matrix to num_rows by num_cols.

- void print (ostream &s) const

  Prints a DakotaMatrix to an output stream.

- void read (UnPackBuffer &s)

  Reads a DakotaMatrix from an UnPackBuffer after an MPI receive.

- void print (PackBuffer &s) const

  Prints a DakotaMatrix to a PackBuffer prior to an MPI send.

- void testClass ()

  Class unit test method.

6.26.1 Detailed Description

template<class T> class DakotaMatrix< T >

Template class for the Dakota numerical matrix.

A matrix class template to provide 2D arrays of objects. The matrix is zero-based, rows: 0 to (numRows-1) and cols: 0 to (numColumns-1). The class supports overloading of the subscript operator allowing it to emulate a normal built-in 2D array type. The DakotaMatrix relies on the DakotaBaseVector template class to manage the differences between the Rogue Wave vector class and the STL vector class.

6.26.2 Member Function Documentation

6.26.2.1 template<class T> DakotaMatrix< T > & DakotaMatrix< T >::operator= (const T & *val*)

Sets all elements in the matrix to ival.

calls base class operator=(ival)

Reimplemented from DakotaBaseVector.

6.26.2.2 template<class T> void DakotaMatrix< T >::testClass ()

Class unit test method.

verifies the basic functionallity of the DakotaMatrix class. The assert function is used to test the correctness of results.

The documentation for this class was generated from the following file:

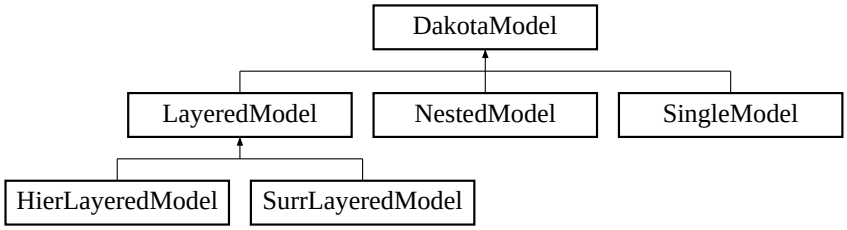
- DakotaMatrix.H

6.27 DakotaModel Class Reference

Base class for the model class hierarchy.

`#include <DakotaModel.H>`

Inheritance diagram for DakotaModel::



Public Methods

- DakotaModel ()
  default constructor.
- DakotaModel (ProblemDescDB &problem_db)
  standard constructor for envelope.
- DakotaModel (const DakotaModel &model)
  copy constructor.
- virtual ~DakotaModel ()
  destructor.
- DakotaModel operator= (const DakotaModel &model)
  assignment operator.
- virtual DakotaModel & subordinate_model ()
  return the sub-model in nested and layered models.
- virtual DakotaIterator & subordinate_iterator ()
  return the sub-iterator in nested and layered models.
- virtual int maximum_concurrency () const
  used to return DACE iterator concurrency for SurrLayeredModels.
- virtual void build_approximation ()
  build the approximation in LayeredModels.
- virtual void update_approximation (const DakotaRealVector &x_star, const DakotaResponse &response_star)

update the approximation in SurrLayeredModels with new data.

- virtual void compute_correction (const DakotaResponse &truth_response, const DakotaResponse &approx_response, const DakotaRealVector &c_vars)

  compute correction factors for use in LayeredModels.

- virtual void auto_correction (short correction_flag)

  manages automatic application of correction factors in LayeredModels.

- virtual void apply_correction (DakotaResponse &approx_response, const DakotaRealVector &c_vars, short quiet_flag=0)

  apply correction factors to approx_response (for use in LayeredModels).

- virtual DakotaString local_eval_synchronization ()

  return derived model synchronization setting.

- virtual void free_communicators ()

  deallocate communicator partitions for a model.

- virtual void serve ()

  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 slave server operations on a particular model when iteration on that model is complete.

- virtual const DakotaIntList & synchronize_nowait_completions ()

  Return completion id's matching response list from synchronize_nowait.

- virtual short derived_master_overload () const

  Return a flag indicating the combination of multiprocessor evaluations and a dedicated master iterator scheduling. Used in synchronous compute_response functions to prevent the error of trying to run a multiprocessor job on the master.

- virtual int total_eval_counter () const

  Return the total evaluation count from the interface.

- virtual int new_eval_counter () const

  Return the new (non-duplicate) evaluation count from the interface.

- void compute_response ()

  Compute the DakotaResponse at currentVariables (default asv).

- void compute_response (const DakotaIntArray &asv)

  Compute the DakotaResponse at currentVariables (specified asv).

- void asynch_compute_response ()

  Spawn an asynchronous job (or jobs) that computes the value of the DakotaResponse at currentVariables (default asv).

- void asynch_compute_response (const DakotaIntArray &asv)

  Spawn an asynchronous job (or jobs) that computes the value of the DakotaResponse at currentVariables (specified asv).

- const DakotaArray< DakotaResponse > & synchronize ()

  Execute a blocking scheduling algorithm to collect the complete set of results from a group of asynchronous evaluations.

- const DakotaList< DakotaResponse > & synchronize_nowait ()

  Execute a nonblocking scheduling algorithm to collect all available results from a group of asynchronous evaluations.

- void init_communicators (const int &max_iterator_concurrency)

  allocate communicator partitions for a model.

- size_t tv () const

  return total number of vars.

- size_t cv () const

  return number of active continuous variables.

- size_t dv () const

  return number of active discrete variables.

- size_t num_functions () const

  return number of functions in currentResponse.

- void active_variables (const DakotaVariables &vars)

  set the active variables in currentVariables.

- const DakotaRealVector & continuous_variables () const

  return the active continuous variables from currentVariables.

- void continuous_variables (const DakotaRealVector &c_vars)

  set the active continuous variables in currentVariables.

- const DakotaIntVector & discrete_variables () const

  return the active discrete variables from currentVariables.

- void discrete_variables (const DakotaIntVector &d_vars)

  set the active discrete variables in currentVariables.

- const DakotaStringArray & continuous_variable_labels () const

  return the active continuous variable labels from currentVariables.

- const DakotaStringArray & discrete_variable_labels () const

  return the active discrete variable labels from currentVariables.

- void inactive_continuous_variables (const DakotaRealVector &i_c_vars)

  set the inactive continuous variables in currentVariables.

- void inactive_discrete_variables (const DakotaIntVector &i_d_vars)
  set the inactive discrete variables in currentVariables.
- const DakotaRealVector & continuous_lower_bounds () const
  return the active continuous variable lower bounds from userDefinedVarConstraints.
- void continuous_lower_bounds (const DakotaRealVector &c_l_bnds)
  set the active continuous variable lower bounds in userDefinedVarConstraints.
- const DakotaRealVector & continuous_upper_bounds () const
  return the active continuous variable upper bounds from userDefinedVarConstraints.
- void continuous_upper_bounds (const DakotaRealVector &c_u_bnds)
  set the active continuous variable upper bounds in userDefinedVarConstraints.
- const DakotaIntVector & discrete_lower_bounds () const
  return the active discrete variable lower bounds from userDefinedVarConstraints.
- void discrete_lower_bounds (const DakotaIntVector &d_l_bnds)
  set the active discrete variable lower bounds in userDefinedVarConstraints.
- const DakotaIntVector & discrete_upper_bounds () const
  return the active discrete variable upper bounds from userDefinedVarConstraints.
- void discrete_upper_bounds (const DakotaIntVector &d_u_bnds)
  set the active discrete variable upper bounds in userDefinedVarConstraints.
- const size_t & num_linear_ineq_constraints () const
  return the number of linear inequality constraints.
- const size_t & num_linear_eq_constraints () const
  return the number of linear equality constraints.
- const DakotaRealMatrix & linear_ineq_constraint_coeffs () const
  return the linear inequality constraint coefficients.
- const DakotaRealVector & linear_ineq_constraint_lower_bounds () const
  return the linear inequality constraint lower bounds.
- const DakotaRealVector & linear_ineq_constraint_upper_bounds () const
  return the linear inequality constraint upper bounds.
- const DakotaRealMatrix & linear_eq_constraint_coeffs () const
  return the linear equality constraint coefficients.
- const DakotaRealVector & linear_eq_constraint_targets () const
  return the linear equality constraint targets.
- const DakotaIntList & merged_integer_list () const

return the list of discrete variables merged into a continuous array in currentVariables.

- const DakotaIntArray & message_lengths () const

  return the array of MPI packed message buffer lengths (messageLengths).

- const DakotaVariables & current_variables () const

  return the current variables (currentVariables).

- const DakotaResponse & current_response () const

  return the current response (currentResponse).

- const ProblemDescDB & prob_desc_db () const

  return the problem description database (probDescDB).

- const DakotaString & model_type () const

  return the model type (modelType).

- short asynch_flag () const

  return the asynchronous evaluation flag (asynchEvalFlag).

- void asynch_flag (const short flag)

  set the asynchronous evaluation flag (asynchEvalFlag).

- void activate_model_auto_graphics ()

  set modelAutoGraphicsFlag to activate posting of graphics data within compute_response/synchronize functions (automatic graphics posting in the model as opposed to graphics posting at the strategy level).

- const DakotaString & gradient_method () const

  return the gradient method (gradType).

- int gradient_concurrency () const

  return the gradient concurrency for use in parallel configuration logic.

- short is_null () const

  function to check modelRep (does this envelope contain a letter).

Protected Methods

- DakotaModel (BaseConstructor, 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).

- virtual void derived_compute_response (const DakotaIntArray &asv)

  portion of compute_response() specific to derived model classes.

- virtual void derived_asynch_compute_response (const DakotaIntArray &asv)

  portion of asynch_compute_response() specific to derived model classes.

- virtual const DakotaArray< DakotaResponse > & derived_synchronize ()

portion of synchronize() specific to derived model classes.

- virtual const DakotaList< DakotaResponse > & derived_synchronize_nowait ()

  portion of synchronize_nowait() specific to derived model classes.

- virtual void derived_init_communicators (const DakotaIntArray &message_lengths, const int &max_iterator_concurrency)

  portion of init_communicators() specific to derived model classes.

Protected Attributes

- DakotaVariables currentVariables

  the set of current variables used by the model for performing function evaluations.

- size_t numGradVars

  the number of active continuous variables (used in the finite difference routines).

- DakotaResponse currentResponse

  the set of current responses that holds the results of model function evaluations.

- size_t numFns

  the number of functions in currentResponse.

- DakotaVarConstraints userDefinedVarConstraints

  Explicit constraints on variables are maintained in the DakotaVarConstraints 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 DakotaResponse since their form and coefficients are published to an iterator at startup.

Private Methods

- DakotaModel * get_model (ProblemDescDB &problem_db)

  Used by the envelope to instantiate the correct letter class.

- int fd_gradients (const DakotaIntArray &map_asv, const DakotaIntArray &fd_grad_asv, const DakotaIntArray &original_asv, const int 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_fd_gradients (const DakotaArray< DakotaResponse > &fd_grad_responses, DakotaResponse &new_response, const DakotaIntArray &fd_grad_asv, const DakotaIntArray &asv)

  combine results from an array of finite difference response objects (fd_grad_responses) into a single response (new_response).

- void update_response (DakotaResponse &new_response, const DakotaIntArray &fd_grad_asv, const DakotaIntArray &asv, const short initial_map, DakotaRealVector &fn_vals_x0, DakotaRealMatrix &partial_fn_grads, const DakotaRealMatrix &new_fn_grads)

overlay results to update a response object.

- void manage_asv (const DakotaIntArray &asv_in, DakotaIntArray &map_asv_out, DakotaIntArray &fd_grad_asv_out, int &use_fd_grad)

  Coordinates map() and fd_gradients() calls given an asv_in input.

Private Attributes

- DakotaModel * modelRep

  pointer to the letter (initialized only for the envelope).

- int referenceCount

  number of objects sharing modelRep.

- const ProblemDescDB & probDescDB

  class member reference to the problem description database.

- const ParallelLibrary & parallelLib

  class member reference to the parallel library.

- DakotaIntArray messageLengths

  length of packed MPI buffers containing vars, vars and asv, response, and PRPair.

- DakotaString modelType

  type of model: single, nested, or layered.

- short asynchFDFlag

  flags use of fd_gradients w/i asynch_compute_response.

- short asynchEvalFlag

  flags asynch evaluations (local or distributed).

- short modelAutoGraphicsFlag

  flag for posting of graphics data within compute_response (automatic graphics posting in the model as opposed to graphics posting at the strategy level).

- DakotaList< DakotaVariables > varsList

  history of vars populated in asynch_compute_response() and used in synchronize().

- DakotaList< DakotaIntArray > asvList

  if asynchFDFlag is set, transfers asv requests to synchronize.

- DakotaShortList initialMapList

  transfers initial_map flag values from fd_gradients to synchronize_fd_gradients.

- DakotaShortList dbFnsList

  transfers db_fns flag values from fd_gradients to synchronize_fd_gradients.

- DakotaList< DakotaResponse > dbResponseList

transfers database captures from fd_gradients to synchronize_fd_gradients.

- DakotaRealList deltaList

  transfers deltas from fd_gradients to synchronize_fd_gradients.

- DakotaIntList numMapsList

  tracks the number of maps used in fd_gradients(). Used in synchronize() as a key for combining finite difference responses into numerical gradients.

- DakotaArray< DakotaResponse > responseArray

  used to return an array of responses for asynchronous evaluations. This array has the responses in final concatenated form. The similar array in DakotaInterface contains the raw responses.

- DakotaList< DakotaResponse > responseList

  used to return a list of responses for asynchronous evaluations. This list has the responses in final concatenated form. The similar list in DakotaInterface contains the raw responses.

- DakotaString gradType

  gradient type: none, numerical, analytic, mixed.

- DakotaString methodSrc

  method source: dakota, vendor.

- DakotaString intervalType

  interval type: forward, central.

- Real finiteDiffSS

  relative finite difference step size.

- DakotaIntList idAnalytic

  analytic fn id's for mixed gradients.

6.27.1 Detailed Description

Base class for the model class hierarchy.

The DakotaModel 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 (DakotaModel) serves as the envelope and one of the derived classes (selected in DakotaModel::get_model()) serves as the letter.

6.27.2 Constructor & Destructor Documentation

6.27.2.1 DakotaModel::DakotaModel ()

default constructor.

The default constructor is used in Vector<DakotaModel> instantiations and for initialization of DakotaModel objects contained in DakotaStrategy derived classes (see derived strategy header files). modelRep is NULL in this case (a populated problem_db is needed to build a meaningful DakotaModel object). This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

6.27.2.2 DakotaModel::DakotaModel (ProblemDescDB & *problem_db*)

standard constructor for envelope.

Used in model instantiations within strategy constructors. Envelope constructor only needs to extract enough data to properly execute get_model, since DakotaModel(BaseConstructor, problem_db) builds the actual base class data for the derived models.

6.27.2.3 DakotaModel::DakotaModel (const DakotaModel & *model*)

copy constructor.

Copy constructor manages sharing of modelRep and incrementing of referenceCount.

6.27.2.4 DakotaModel::~DakotaModel () [virtual]

destructor.

Destructor decrements referenceCount and only deletes modelRep when referenceCount reaches zero.

6.27.2.5 DakotaModel::DakotaModel (BaseConstructor, 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 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 (an uninitialized pointer causes problems in ~DakotaModel).

6.27.3 Member Function Documentation

6.27.3.1 DakotaModel DakotaModel::operator= (const DakotaModel & *model*)

assignment operator.

Assignment operator decrements referenceCount for old modelRep, assigns new modelRep, and increments referenceCount for new modelRep.

6.27.3.2 DakotaString DakotaModel::local_eval_synchronization () [virtual]

return derived model synchronization setting.

SingleModels and HierLayeredModels 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. Also, probDescDB "interface.synchronization" will be bad if no optional interface (will contain last interface spec. parsed).
- SurrLayeredModels: while asynch evals on approximations will work due to some added bookkeeping, avoiding them is preferable.

Reimplemented in HierLayeredModel, and SingleModel.

6.27.3.3 void DakotaModel::init_communicators (const int & *max_iterator_concurrency*)

allocate communicator partitions for a model.

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.

6.27.3.4 DakotaModel * DakotaModel::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.

6.27.3.5 int DakotaModel::fd_gradients (const DakotaIntArray & *map_asv*, const DakotaIntArray & *fd_grad_asv*, const DakotaIntArray & *original_asv*, const int *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.

Compute finite difference gradients, put the data in currentResponse, and return the number of maps used by fd_gradients. This return value is used by asynch_compute_response() and synchronize() to track response arrays and it could be used to improve management of max_function_evaluations within the iterators.

6.27.3.6 void DakotaModel::synchronize_fd_gradients (const DakotaArray< DakotaResponse > & *fd_grad_responses*, DakotaResponse & *new_response*, const DakotaIntArray & *fd_grad_asv*, const DakotaIntArray & *asv*) [private]

combine results from an array of finite difference response objects (fd_grad_responses) into a single response (new_response).

Merge a vector of fd_grad_responses into a single new_response. This function is used both by compute_response() for the case of asynchronous fd_gradients() and by synchronize() for the case where one or more asynch_compute_response() calls has employed asynchronous fd_gradients().

6.27.3.7 void DakotaModel::update_response (DakotaResponse & *new_response*, const DakotaIntArray & *fd_grad_asv*, const DakotaIntArray & *asv*, const short *initial_map*, DakotaRealVector & *fn_vals_x0*, DakotaRealMatrix & *partial_fn_grads*, const DakotaRealMatrix & *new_fn_grads*) [private]

overlay results to update a response object.

Overlay function value and numerical gradient data to populate new_response as governed by initial_map flag and asv vectors. If initial_map occurred, then add to the partial response object created by the map. If initial_map was not used, then only new_fn_grads should be present in the updated new_response. Convenience function used by fd_gradients for the synchronous case and by synchronize_fd_gradients for the asynchronous case.

6.27.3.8 void DakotaModel::manage_asv (const DakotaIntArray & *asv_in*, DakotaIntArray & *map_asv_out*, DakotaIntArray & *fd_grad_asv_out*, int & *use_fd_grad*) [private]

Coordinates map() and fd_gradients() calls given an asv_in input.

Splits asv_in total request into map_asv_out for use by map() and fd_grad_asv_out for use by fd_gradients(), as governed by gradient specification.

The documentation for this class was generated from the following files:

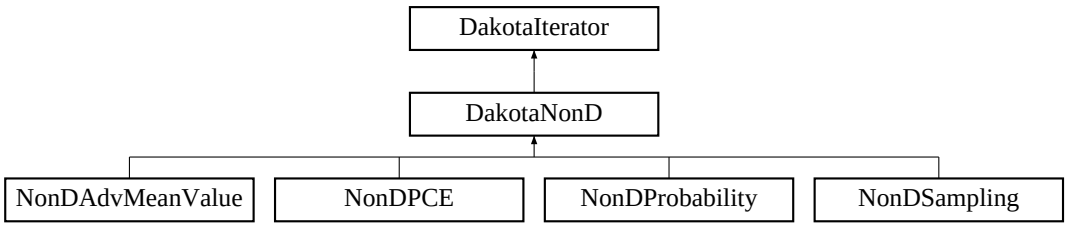
- DakotaModel.H
- DakotaModel.C

6.28 DakotaNonD Class Reference

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

`#include <DakotaNonD.H>`

Inheritance diagram for DakotaNonD::



Protected Methods

- DakotaNonD (DakotaModel &model)

  constructor.

- DakotaNonD (NoDBBaseConstructor, DakotaModel &model)

  alternate constructor for instantiations "on the fly".

- ~DakotaNonD ()

  destructor.

- void run_iterator ()

  redefines the main iterator hierarchy virtual function to invoke quantify_uncertainty.

- virtual void quantify_uncertainty ()=0

  performs a forward uncertainty propagation of parameter distributions into response statistics.

- void vector_statistics (int num_ran_var, int num_obs, const DakotaRealVectorArray &samples, const DakotaRealArray &thresh)

  computes mean, standard deviation, and probability of threshold exceedance for the samples input, where samples may be input or output-related.

- const DakotaResponse & iterator_response_results () const

  return the final statistics from the nondeterministic iteration.

Protected Attributes

- DakotaRealVector normalMeans

  normal uncertain variable means.

- DakotaRealVector normalStdDevs
  normal uncertain variable standard deviations.
- DakotaRealVector normalDistLowerBnds
  normal uncertain variable distribution lower bounds.
- DakotaRealVector normalDistUpperBnds
  normal uncertain variable distribution upper bounds.
- DakotaRealVector lognormalMeans
  lognormal uncertain variable means.
- DakotaRealVector lognormalStdDevs
  lognormal uncertain variable standard deviations.
- DakotaRealVector lognormalErrFacts
  lognormal uncertain variable error factors.
- DakotaRealVector lognormalDistLowerBnds
  lognormal uncertain variable distribution lower bounds.
- DakotaRealVector lognormalDistUpperBnds
  lognormal uncertain variable distribution upper bounds.
- DakotaRealVector uniformDistLowerBnds
  uniform uncertain variable distribution lower bounds.
- DakotaRealVector uniformDistUpperBnds
  uniform uncertain variable distribution upper bounds.
- DakotaRealVector loguniformDistLowerBnds
  loguniform uncertain variable distribution lower bounds.
- DakotaRealVector loguniformDistUpperBnds
  loguniform uncertain variable distribution upper bounds.
- DakotaRealVector weibullAlphas
  weibull uncertain variable alphas.
- DakotaRealVector weibullBetas
  weibull uncertain variable betas.
- DakotaStringList histogramFilenames
  histogram uncertain variable filenames.
- DakotaRealMatrix uncertainCorrelations
  uncertain variable correlation matrix (rank correlations for sampling and correlation coefficients for analytic reliability).
- size_t numNormalVars

number of normal uncertain variables.

- size_t numLognormalVars

  number of lognormal uncertain variables.

- size_t numUniformVars

  number of uniform uncertain variables.

- size_t numLoguniformVars

  number of loguniform uncertain variables.

- size_t numWeibullVars

  number of weibull uncertain variables.

- size_t numHistogramVars

  number of histogram uncertain variables.

- size_t numUncertainVars

  total number of uncertain variables.

- size_t numResponseFunctions

  number of response functions.

- DakotaRealVector meanStats

  means computed in vector_statistics().

- DakotaRealVector stdDevStats

  std deviations computed in vector_statistics().

- DakotaRealVector probMoreThanThresh

  probabilities that response functions are greater than respThresh (computed in vector_statistics()).

- DakotaResponse finalStatistics

  final statistics from the forward uncertainty propagation: response means, response standard deviations, probabilities of failure.

- short correlationFlag

  flag for indicating if correlation exists among the uncertain variables.

6.28.1 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.

The documentation for this class was generated from the following files:

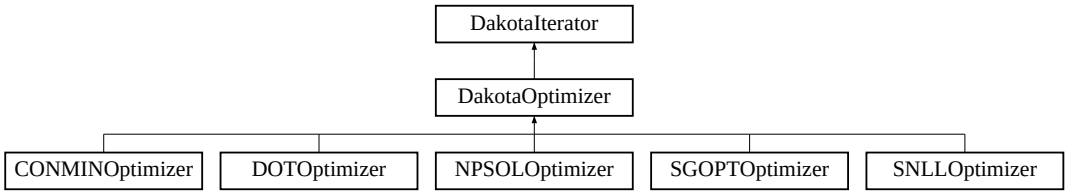
- DakotaNonD.H
- DakotaNonD.C

6.29 DakotaOptimizer Class Reference

Base class for the optimizer branch of the iterator hierarchy.

`#include <DakotaOptimizer.H>`

Inheritance diagram for DakotaOptimizer::



Public Methods

- void run_iterator ()

  run the iterator.

- const DakotaVariables & iterator_variable_results () const

  return the final iterator solution (variables).

- const DakotaResponse & iterator_response_results () const

  return the final iterator solution (response).

- void print_iterator_results (ostream &s) const
- void multi_objective_weights (const DakotaRealVector &multi_obj_wts)

  set the relative weightings for multiple objective functions. Used by ConcurrentStrategy for Pareto set optimization.

Protected Methods

- DakotaOptimizer ()

  default constructor.

- DakotaOptimizer (DakotaModel &model)

  standard constructor.

- ~DakotaOptimizer ()

  destructor.

- virtual void find_optimum ()=0

  Used within the optimizer branch for computing the optimal solution. Redefines the run_iterator virtual function for the optimizer branch.

Static Protected Methods

- DakotaResponse multi_objective_modify (const DakotaResponse &raw_response)
  maps multiple objective functions to a single objective for single-objective optimizers.

Protected Attributes

- int realWorkSpaceSize
  size of realWorkSpace.
- int intWorkSpaceSize
  size of intWorkSpace.
- DakotaRealArray realWorkSpace
  real work space for f77 optimizers.
- DakotaIntArray intWorkSpace
  int work space for f77 optimizers.
- size_t numObjectiveFunctions
  number of objective functions.
- Real convergenceTol
  optimizer convergence tolerance.
- Real constraintTol
  optimizer constraint tolerance.
- size_t numNonlinearIneqConstraints
  number of nonlinear inequality constraints.
- DakotaRealVector nonlinearIneqLowerBnds
  nonlinear inequality constraint lower bounds.
- DakotaRealVector nonlinearIneqUpperBnds
  nonlinear inequality constraint upper bounds.
- Real bigBoundSize
  cutoff value for inequality constraint bounds.
- size_t numNonlinearEqConstraints
  number of nonlinear equality constraints.
- DakotaRealVector nonlinearEqTargets
  nonlinear equality constraint targets.
- int numNonlinearConstraints
  total number of nonlinear constraints.

- int numConstraints

  total number of linear and nonlinear constraints (for DOT/CONMIN).

- size_t numLinearIneqConstraints

  number of linear inequality constraints.

- DakotaRealMatrix linearIneqConstraintCoeffs

  linear inequality constraint coefficients.

- DakotaRealVector linearIneqLowerBnds

  linear inequality constraint lower bounds.

- DakotaRealVector linearIneqUpperBnds

  linear inequality constraint upper bounds.

- size_t numLinearEqConstraints

  number of linear equality constraints.

- DakotaRealMatrix linearEqConstraintCoeffs

  linear equality constraint coefficients.

- DakotaRealVector linearEqTargets

  linear equality constraint targets.

- int numLinearConstraints

  total number of linear constraints.

- int localConstraintArraySize

  used by Fortran optimizers for non-zero array sizing.

- short speculativeFlag

  flag for speculative optimization approach.

- short vendorNumericalGradFlag

  convenience flag for gradType==”numerical” && methodSource==”vendor”.

- DakotaVariables bestVariables

  best variables found by optimizer.

- DakotaResponse bestResponses

  best response found by optimizer.

Static Protected Attributes

- size_t staticNumContinuousVars

  static copy of numContinuousVars used in static functions passed by function pointer (NPSOL and OPT++).

- size_t staticNumObjFns

static copy of numObjectiveFns used in static functions passed by function pointer (NPSOL and OPT++).

- size_t staticNumNonlinearConstraints

  static copy of numNonlinearConstraints used in static functions passed by function pointer (NPSOL and OPT++).

Private Attributes

- DakotaRealVector multiObjWeights

  user-specified weights for multiple objective functions.

Static Private Attributes

- DakotaRealVector staticMultiObjWeights

  static copy of multiObjWeights used in static functions passed by function pointer (NPSOL and OPT++).

6.29.1 Detailed Description

Base class for the optimizer branch of the iterator hierarchy.

The DakotaOptimizer class provides common data and functionality for DOTOptimizer, NPSOLOptimizer, SNLLOptimizer, and SGOPTOptimizer.

6.29.2 Constructor & Destructor Documentation

6.29.2.1 DakotaOptimizer::DakotaOptimizer (DakotaModel & *model*) [protected]

standard constructor.

This constructor extracts the inherited data for the optimizer branch and performs sanity checking on gradient and constraint settings.

6.29.3 Member Function Documentation

6.29.3.1 void DakotaOptimizer::run_iterator () [virtual]

run the iterator.

This function is the primary run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from DakotaIterator.

6.29.3.2 void DakotaOptimizer::print_iterator_results (ostream & *s*) const [virtual]

Redefines default iterator results printing to include optimization results (objective function and constraints).

Reimplemented from DakotaIterator.

6.29.3.3 DakotaResponse DakotaOptimizer::multi_objective_modify (const DakotaResponse & *raw_response*) [static, protected]

maps multiple objective functions to a single 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 staticMultiObjWeights) is the only technique supported currently. The weightings are used to scale function values, gradients, and Hessians as needed.

The documentation for this class was generated from the following files:

- DakotaOptimizer.H
- DakotaOptimizer.C

6.30 DakotaResponse Class Reference

Container class for response functions and their derivatives. DakotaResponse provides the handle class.

`#include <DakotaResponse.H>`

Public Methods

- DakotaResponse ()
  default constructor.
- DakotaResponse (int num_params, const ProblemDescDB &problem_db)
  standard constructor built from problem description database.
- DakotaResponse (int num_params, const DakotaIntArray &asv)
  alternate constructor using limited data.
- DakotaResponse (const DakotaResponse &response)
  copy constructor.
- ~DakotaResponse ()
  destructor.
- DakotaResponse operator= (const DakotaResponse &response)
  assignment operator.
- int operator== (const DakotaResponse &response) const
  equality operator.
- size_t num_functions () const
  return the number of response functions.
- const DakotaIntArray & active_set_vector () const
  return the active set vector.
- void active_set_vector (const DakotaIntArray &asv)
  set the active set vector.
- const DakotaString & interface_id () const
  return the interface identifier.
- void interface_id (const DakotaString &id)
  set the interface identifier.
- const DakotaStringArray & fn_tags () const
  return the function identifier strings.

- void fn_tags (const DakotaStringArray &tags)
  set the function identifier strings.
- const DakotaRealVector & function_values () const
  return the function values.
- void function_values (const DakotaRealVector &function_vals)
  set the function values.
- const DakotaRealMatrix & function_gradients () const
  return the function gradients.
- void function_gradients (const DakotaRealMatrix &function_grads)
  set the function gradients.
- const DakotaRealMatrixArray & function_hessians () const
  return the function Hessians.
- void function_hessians (const DakotaRealMatrixArray &function_hessians)
  set the function Hessians.
- void read (istream &s)
  read a response object from an istream.
- void write (ostream &s) const
  write a response object to an ostream.
- void read_annotated (istream &s)
  read a response object in annotated format from an istream.
- void write_annotated (ostream &s) const
  write a response object in annotated format to an ostream.
- void write_tabular (ostream &s) const
  write responseRep::functionValues in tabular format to an ostream.
- void read (DakotaBiStream &s)
  read a response object from the binary restart stream.
- void write (DakotaBoStream &s) const
  write a response object to the binary restart stream.
- void read (UnPackBuffer &s)
  read a response object from a packed MPI buffer.
- void write (PackBuffer &s) const
  write a response object to a packed MPI buffer.
- DakotaResponse copy () const
  a deep copy for use in history mechanisms.

- int data_size ()

  handle class forward to corresponding body class member function.

- void read_data (double *response_data)

  handle class forward to corresponding body class member function.

- void write_data (double *response_data)

  handle class forward to corresponding body class member function.

- void overlay (const DakotaResponse &response)

  handle class forward to corresponding body class member function.

- void copy_results (const DakotaResponse &response)

  handle class forward to corresponding body class member function.

- void purge_inactive ()

  handle class forward to corresponding body class member function.

- void reset ()

  handle class forward to corresponding body class member function.

Private Attributes

- DakotaResponseRep * responseRep

  pointer to the body (handle-body idiom).

6.30.1 Detailed Description

Container class for response functions and their derivatives. DakotaResponse provides the handle class.

The DakotaResponse 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). It is not currently part of a class hierarchy, since the abstraction has been sufficiently general and has not required specialization. For memory efficiency, it employs the "handle-body idiom" approach to reference counting and representation sharing (see Coplien "Advanced C++", p. 58), for which DakotaResponse serves as the handle and DakotaResponseRep serves as the body.

6.30.2 Constructor & Destructor Documentation

6.30.2.1 DakotaResponse::DakotaResponse ()

default constructor.

Need a populated problem description database to build a meaningful DakotaResponse object, so set the responseRep=NULL in default constructor for efficiency. This then requires a check on NULL in the copy constructor, assignment operator, and destructor.

The documentation for this class was generated from the following files:

- DakotaResponse.H
- DakotaResponse.C

6.31 DakotaResponseRep Class Reference

Container class for response functions and their derivatives. DakotaResponseRep provides the body class.

`#include <DakotaResponse.H>`

Private Methods

- DakotaResponseRep ()
  default constructor.
- DakotaResponseRep (int num_params, const ProblemDescDB &problem_db)
  standard constructor built from problem description database.
- DakotaResponseRep (int num_params, const DakotaIntArray &asv)
  alternate constructor using limited data.
- ~DakotaResponseRep ()
  destructor.
- void read (istream &s)
  read a responseRep object from an istream.
- void write (ostream &s) const
  write a responseRep object to an ostream.
- void read_annotated (istream &s)
  read a responseRep object from an istream (annotated format).
- void write_annotated (ostream &s) const
  write a responseRep object to an ostream (annotated format).
- void write_tabular (ostream &s) const
  write functionValues to an ostream (tabular format).
- void read (DakotaBiStream &s)
  read a responseRep object from a binary stream.
- void write (DakotaBoStream &s) const
  write a responseRep object to a binary stream.
- void read (UnPackBuffer &s)
  read a responseRep object from a packed MPI buffer.
- void write (PackBuffer &s) const
  write a responseRep object to a packed MPI buffer.

- 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 DakotaResponse &response)

  add incoming response to functionValues/Gradients/Hessians.

- void copy_results (const DakotaResponse &response)

  copy functionValues, functionGradients, & functionHessians data only. Do not copy ASV, tags, id's, etc. Used in place of assignment operator for retrieving results data from the data_pairs list without corrupting other data.

- void purge_inactive ()

  Purge extraneous data from the response object (used when a response object is returned from the database (desired_pair) with more data than needed by the search_pair ASV (see ApplicationInterface::map and DakotaModel::fd_gradients).

- void reset ()

  resets functionValues, functionGradients, and functionHessians to zero.

Private Attributes

- int referenceCount

  number of handle objects sharing responseRep.

- DakotaRealVector functionValues

  abstract set of functions.

- DakotaRealMatrix functionGradients

  first derivatives.

- DakotaRealMatrixArray functionHessians

  second derivatives.

- DakotaIntArray responseASV

  Copy of DakotaIterator's activeSetVector needed for operator overloaded I/O.

- DakotaStringArray fnTags

  function identifiers used to improve output readability.

- DakotaString interfaceId

  the interface used to generate this response object. Used in PRPair::vars_asv_compare.

Friends

- class DakotaResponse

  the handle class can access attributes of the body class directly.

6.31.1 Detailed Description

Container class for response functions and their derivatives. DakotaResponseRep provides the body class.

The DakotaResponseRep 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 (DakotaResponse) provides for memory efficiency in management of multiple response objects through reference counting and representation sharing. The body class (DakotaResponseRep) actually contains the response data (functionValues, functionGradients, functionHessians, etc.). The representation is hidden in that an instance of DakotaResponseRep may only be created by DakotaResponse. Therefore, programmers create instances of the DakotaResponse 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).

6.31.2 Constructor & Destructor Documentation

6.31.2.1 DakotaResponseRep::DakotaResponseRep (int *num_params*, const ProblemDescDB & *problem_db*) [private]

standard constructor built from problem description database.

The standard constructor used by DakotaModelRep. An interfaceId identifies a set of results with the interface used in generating them, which allows vars_asv_compare to prevent duplicate detection on results from different interfaces.

6.31.2.2 DakotaResponseRep::DakotaResponseRep (int *num_params*, const DakotaIntArray & *asv*) [private]

alternate constructor using limited data.

Used for building a response object of the correct size on the fly (e.g., by slave analysis servers performing execute() on a local_response). fnTags and interfaceId are not needed for this purpose since they're not passed in the MPI send/recv buffers (NOTE: if interfaceId becomes needed, it could be set from an AppInt attribute passed from AppInt::serve()). However, NPSOLOptimizer's user-defined functions option uses this constructor to build bestResponses and bestResponses needs fnTags for I/O, so construction of fnTags has been added.

6.31.3 Member Function Documentation

6.31.3.1 void DakotaResponseRep::read (istream & *s*) [private]

read a responseRep object from an istream.

ASCII version of read needs capabilities for capturing data omissions or formatting errors (resulting from user error or asynch race condition) and analysis failures (resulting from nonconvergence, instability, etc.).

6.31.3.2 void DakotaResponseRep::write (ostream & *s*) const [private]

write a responseRep object to an ostream.

ASCII version of write.

6.31.3.3 void DakotaResponseRep::read_annotated (istream & *s*) [private]

read a responseRep object from an istream (annotated format).

read_annotated version is used for neutral file translation of restart files. Since objects are built solely from this data, annotations are used. This version is currently identical to the DakotaBiStream version.

6.31.3.4 void DakotaResponseRep::write_annotated (ostream & *s*) const [private]

write a responseRep object to an ostream (annotated format).

write_annotated version is used for neutral file translation of restart files. Since objects need to be build solely from this data, annotations are used. This version differs from the DakotaBoStream version only in the use of white space between fields.

6.31.3.5 void DakotaResponseRep::write_tabular (ostream & *s*) const [private]

write functionValues to an ostream (tabular format).

write_tabular is used for output of functionValues in a tabular format for convenience in post-processing/plotting of DAKOTA results. Objects are not built from this data (there is no corresponding read_tabular).

6.31.3.6 void DakotaResponseRep::read (DakotaBiStream & *s*) [private]

read a responseRep object from a binary stream.

Binary version differs from ASCII version in 2 primary ways: (1) it lacks formatting. (2) the DakotaResponse has not been sized a priori. In reading data from the binary restart file, a ParamResponsePair was constructed with its default constructor which called the DakotaResponse default constructor. Therefore, we must first read sizing data and resize the arrays.

6.31.3.7 void DakotaResponseRep::write (DakotaBoStream & *s*) const [private]

write a responseRep object to a binary stream.

Binary version differs from ASCII version in 2 primary ways: (1) It lacks formatting. (2) In reading data from the binary restart file, ParamResponsePairs are constructed with their default constructor which calls

the DakotaResponse default constructor. Therefore, we must first write sizing data so that DakotaResponse-Rep::read(DakotaBoStream& s) can resize the arrays.

6.31.3.8 void DakotaResponseRep::read (UnPackBuffer & *s*) [private]

read a responseRep object from a packed MPI buffer.

UnpackBuffer version differs from DakotaBiStream version only in omission of interfaceId and default fnTags. Master processor retains tags and ids and communicates asv and response data only with slaves.

6.31.3.9 void DakotaResponseRep::write (PackBuffer & *s*) const [private]

write a responseRep object to a packed MPI buffer.

PackBuffer version differs from DakotaBoStream version only in omissions of interfaceId and flush. The master processor retains tags and ids and communicates asv and response data only with slaves.

The documentation for this class was generated from the following files:

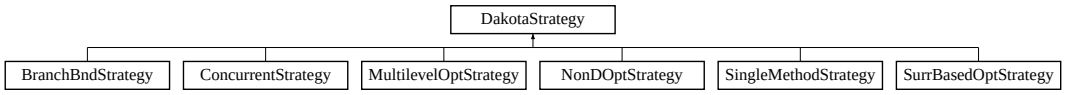
- DakotaResponse.H
- DakotaResponse.C

6.32 DakotaStrategy Class Reference

Base class for the strategy class hierarchy.

`#include <DakotaStrategy.H>`

Inheritance diagram for DakotaStrategy::



Public Methods

- DakotaStrategy ()

  default constructor (should not be used).

- DakotaStrategy (ProblemDescDB &problem_db)

  constructor.

- DakotaStrategy (const DakotaStrategy &strat)

  copy constructor.

- virtual ~DakotaStrategy ()

  destructor.

- DakotaStrategy operator= (const DakotaStrategy &strat)

  assignment operator.

- virtual void run_strategy ()

  the run function for the strategy: invoke the iterator(s) on the model(s). Called from main.C.

- void run_iterator (DakotaIterator &the_iterator, DakotaModel &the_model)

  Convenience function for invoking an iterator on a model and managing parallelism. Function must be public due to use by MINLPNode.

- MPI_Comm iterator_communicator () const

  return iteratorComm (used only by MINLPNode).

- int iterator_communicator_size () const

  return iteratorCommSize (used only by MINLPNode).

Protected Methods

- DakotaStrategy (BaseConstructor, 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).

- void initialize_graphics (const DakotaModel &model)

  convenience function for initialization of 2D graphics and data tabulation.

Protected Attributes

- ProblemDescDB & probDescDB

  class member reference to the problem description database.

- ParallelLibrary & parallelLib

  class member reference to the parallel library.

- DakotaString strategyName

  type of strategy: single_method, multi_level, surrogate_based_opt, opt_under_uncertainty, branch_and_bound, multi_start, or pareto_set.

- int worldRank

  processor rank in MPI_COMM_WORLD.

- int worldSize

  size of MPI_COMM_WORLD.

- MPI_Comm iteratorComm

  the communicator defining the group of processors on which an iterator executes. Results from init_iterator_comms.

- int iteratorCommRank

  processor rank in iteratorComm.

- int iteratorCommSize

  number of processors in iteratorComm.

- short graphicsFlag

  flag for using graphics in a graphics executable.

- short tabularDataFlag

  flag for file tabulation of graphics data.

- DakotaString tabularDataFile

  filename for tabulation of graphics data.

Private Methods

- DakotaStrategy * get_strategy (ProblemDescDB &problem_db)

  Used by the envelope to instantiate the correct letter class.

- ProblemDescDB & prob_desc_db () const

  returns the problem description database (probDescDB).

Private Attributes

- DakotaStrategy * strategyRep

  pointer to the letter (initialized only for the envelope).

- int referenceCount

  number of objects sharing strategyRep.

6.32.1 Detailed Description

Base class for the strategy class hierarchy.

The DakotaStrategy class is the base class for the class hierarchy providing the top level control in DAKOTA. The strategy is responsible for creating and managing iterators and models. For memory efficiency and enhanced polymorphism, the strategy hierarchy employs the "letter/envelope idiom" (see Coplien "Advanced C++", p. 133), for which the base class (DakotaStrategy) serves as the envelope and one of the derived classes (selected in DakotaStrategy::get_strategy()) serves as the letter.

6.32.2 Constructor & Destructor Documentation

6.32.2.1 DakotaStrategy::DakotaStrategy ()

default constructor (should not be used).

The default constructor should not be used. strategyRep is NULL in this case (a populated problem_db is needed to build a meaningful DakotaStrategy object). This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

6.32.2.2 DakotaStrategy::DakotaStrategy (ProblemDescDB & *problem_db*)

constructor.

Used in main.C instantiation to build the envelope. This constructor only needs to extract enough data to properly execute get_strategy, since DakotaStrategy::DakotaStrategy(BaseConstructor, problem_db) builds the actual base class data inherited by the derived strategies.

6.32.2.3 DakotaStrategy::DakotaStrategy (const DakotaStrategy & *strat*)

copy constructor.

Copy constructor manages sharing of strategyRep and incrementing of referenceCount.

6.32.2.4 DakotaStrategy::~DakotaStrategy () [virtual]

destructor.

Destructor decrements referenceCount and only deletes strategyRep when referenceCount reaches zero.

6.32.2.5 DakotaStrategy::DakotaStrategy (BaseConstructor, 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 strategies. get_strategy() 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_strategy() again). Since the letter IS the representation, its representation pointer is set to NULL (an uninitialized pointer causes problems in ~DakotaStrategy).

6.32.3 Member Function Documentation

6.32.3.1 DakotaStrategy DakotaStrategy::operator= (const DakotaStrategy & *strat*)

assignment operator.

Assignment operator decrements referenceCount for old strategyRep, assigns new strategyRep, and increments referenceCount for new strategyRep.

6.32.3.2 void DakotaStrategy::run_iterator (DakotaIterator & *the_iterator*, DakotaModel & *the_model*)

Convenience function for invoking an iterator on a model and managing parallelism. Function must be public due to use by MINLPNode.

This is a convenience function for encapsulating the parallel features (init/serve/etc.) of running an iterator. It does not require a strategyRep forward since it is only used by letter objects. While it is currently a public function due to its use in MINLPNode, this usage still involves a strategy letter object.

6.32.3.3 void DakotaStrategy::initialize_graphics (const DakotaModel & *model*) [protected]

convenience function for initialization of 2D graphics and data tabulation.

This is a convenience function for encapsulating graphics initialization operations. It is not a public function for which a strategyRep forward would be needed, rather it is used exclusively by letter objects.

6.32.3.4 DakotaStrategy * DakotaStrategy::get_strategy (ProblemDescDB & *problem_db*) [private]

Used by the envelope to instantiate the correct letter class.

Used only by the envelope constructor to initialize strategyRep to the appropriate derived type, as given by the strategyName attribute.

6.32.3.5 ProblemDescDB & DakotaStrategy::prob_desc_db () const [inline, private]

returns the problem description database (probDescDB).

Used only by the copy constructor (otherwise strategyRep forward needed).

The documentation for this class was generated from the following files:

- DakotaStrategy.H
- DakotaStrategy.C

6.33 DakotaString Class Reference

DakotaString class, used as main string class for Dakota.

`#include <DakotaString.H>`

Public Methods

- DakotaString ()
  Default constructor.
- DakotaString (const DakotaString &a)
  Default copy constructor.
- DakotaString (const char *initial_val)
  Copy constructor from standard C char array.
- ~DakotaString ()
  Destructor.
- void testClass ()
  Class unit test method.
- DakotaString & toUpper ()
  Convert to upper case string.
- void upper ()
- DakotaString & toLower ()
  Convert to lower case string.
- void lower ()
- bool contains (const char *subString) const
  Returns true if DakotaString contains char substring.*
- bool isNull () const
  Returns true of DakotaString is empty.
- char * data () const
  Returns pointer to standard C char array.
- DakotaString & operator= (const DakotaString &)
  Normal assignment operator.
- DakotaString & operator= (const DAKOTA_BASE_STRING &)
  Assignment operator for base string.
- DakotaString & operator= (const char *)

Assignment operator, standard C char∗.

- operator const char ∗ () const

  The operator() returns pointer to standard C char array.

6.33.1 Detailed Description

DakotaString class, used as main string class for Dakota.

The DakotaString class is the common string class for Dakota. It provides a common interface for string operations whether inheriting from the STL basic_string or the Rogue Wave RWCString class

6.33.2 Member Function Documentation

6.33.2.1 void DakotaString::testClass ()

Class unit test method.

Unit test method for the DakotaString class. Provides a quick way to test the basic functionallity of the class. Utilizes the assert function to test for correctness, will abort if an unexpected answer is received.

6.33.2.2 void DakotaString::upper ()

Private method which converts DakotaString to upper. Utilizes a STL iterator to step through the string and then calls the STL toupper() method. Needs to be done this way because STL only provides a single char toupper method.

6.33.2.3 void DakotaString::lower ()

Private method which converts DakotaString to lower. Utilizes a STL iterator to step through the string and then calls the STL tolower() method. Needs to be done this way because STL only provides a single char tolower method.

6.33.2.4 bool DakotaString::contains (const char ∗ *subString*) const

Returns true if DakotaString contains char∗ substring.

Returns true of the DakotaString contains the char∗ subString. Calls the STL rfind() method, then checks if substring was found within the DakotaString

6.33.2.5 char ∗ DakotaString::data () const

Returns pointer to standard C char array.

Returns a pointer to c style char array. Needed to mimick the Rogue Wave string class. USE WITH CARE.

6.33.2.6 DakotaString::operator const char * () const

The operator() returns pointer to standard C char array.

The operator() returns a pointer to a char string. Uses the STL c_str() method. This allows for the DakotaString to be used in method calls without having to call the data() or c_str() methods.

The documentation for this class was generated from the following files:

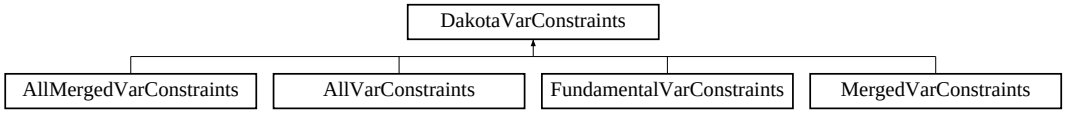
- DakotaString.H
- DakotaString.C

6.34 DakotaVarConstraints Class Reference

Base class for the variable constraints class hierarchy.

`#include <DakotaVarConstraints.H>`

Inheritance diagram for DakotaVarConstraints::



Public Methods

- DakotaVarConstraints ()
  default constructor.
- DakotaVarConstraints (const ProblemDescDB &problem_db, const DakotaString &vars_type)
  standard constructor.
- DakotaVarConstraints (const DakotaVarConstraints &vc)
  copy constructor.
- virtual ~DakotaVarConstraints ()
  destructor.
- DakotaVarConstraints operator= (const DakotaVarConstraints &vc)
  assignment operator.
- virtual const DakotaRealVector & continuous_lower_bounds () const
  return the active continuous variable lower bounds.
- virtual void continuous_lower_bounds (const DakotaRealVector &c_l_bnds)
  set the active continuous variable lower bounds.
- virtual const DakotaRealVector & continuous_upper_bounds () const
  return the active continuous variable upper bounds.
- virtual void continuous_upper_bounds (const DakotaRealVector &c_u_bnds)
  set the active continuous variable upper bounds.
- virtual const DakotaIntVector & discrete_lower_bounds () const
  return the active discrete variable lower bounds.
- virtual void discrete_lower_bounds (const DakotaIntVector &d_l_bnds)
  set the active discrete variable lower bounds.

- virtual const DakotaIntVector & discrete_upper_bounds () const

  return the active discrete variable upper bounds.

- virtual void discrete_upper_bounds (const DakotaIntVector &d_u_bnds)

  set the active discrete variable upper bounds.

- virtual void write (ostream &s) const

  write a variable constraints object to an ostream.

- virtual void read (istream &s)

  read a variable constraints object from an istream.

- const size_t & num_linear_ineq_constraints () const

  return the number of linear inequality constraints.

- const size_t & num_linear_eq_constraints () const

  return the number of linear equality constraints.

- const DakotaRealMatrix & linear_ineq_constraint_coeffs () const

  return the linear inequality constraint coefficients.

- const DakotaRealVector & linear_ineq_constraint_lower_bounds () const

  return the linear inequality constraint lower bounds.

- const DakotaRealVector & linear_ineq_constraint_upper_bounds () const

  return the linear inequality constraint upper bounds.

- const DakotaRealMatrix & linear_eq_constraint_coeffs () const

  return the linear equality constraint coefficients.

- const DakotaRealVector & linear_eq_constraint_targets () const

  return the linear equality constraint targets.

Protected Methods

- DakotaVarConstraints (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).

- void manage_linear_constraints (const ProblemDescDB &problem_db, const size_t &num_vars)

  perform checks on user input, convert linear constraint coefficient input to matrices, and assign defaults.

- size_t num_active_variables () const

  return number of active variables.

Protected Attributes

- DakotaString variablesType

  All, Merged, AllMerged, or Fundamental.

- short discreteFlag

  flags discrete variable mode.

- size_t numLinearIneqConstraints

  number of linear inequality constraints.

- size_t numLinearEqConstraints

  number of linear equality constraints.

- DakotaRealMatrix linearIneqConstraintCoeffs

  linear inequality constraint coefficients.

- DakotaRealMatrix linearEqConstraintCoeffs

  linear equality constraint coefficients.

- DakotaRealVector linearIneqConstraintLowerBnds

  linear inequality constraint lower bounds.

- DakotaRealVector linearIneqConstraintUpperBnds

  linear inequality constraint upper bounds.

- DakotaRealVector linearEqConstraintTargets

  linear equality constraint targets.

Private Methods

- DakotaVarConstraints * get_var_constraints (const ProblemDescDB &problem_db)

  Used only by the constructor to initialize varConstraintsRep to the appropriate derived type.

Private Attributes

- DakotaVarConstraints * varConstraintsRep

  pointer to the letter (initialized only for the envelope).

- int referenceCount

  number of objects sharing varConstraintsRep.

6.34.1 Detailed Description

Base class for the variable constraints class hierarchy.

The DakotaVarConstraints class is the base class for the class hierarchy managing linear and bound constraints on the variables. Using the variable lower and upper bounds arrays and linear constraint coefficients and bounds from the input specification, different derived classes define different views of this data. 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 (DakotaVarConstraints) serves as the envelope and one of the derived classes (selected in DakotaVarConstraints::get_var_constraints()) serves as the letter.

6.34.2 Constructor & Destructor Documentation

6.34.2.1 DakotaVarConstraints::DakotaVarConstraints ()

default constructor.

The default constructor: varConstraintsRep is NULL in this case (a populated problem_db is needed to build a meaningful DakotaVarConstraints object). This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

6.34.2.2 DakotaVarConstraints::DakotaVarConstraints (const ProblemDescDB & *problem_db*, const DakotaString & *vars_type*)

standard constructor.

The envelope constructor only needs to extract enough data to properly execute get_var_constraints, since the constructor overloaded with BaseConstructor builds the actual base class data inherited by the derived classes.

6.34.2.3 DakotaVarConstraints::DakotaVarConstraints (const DakotaVarConstraints & *vc*)

copy constructor.

Copy constructor manages sharing of varConstraintsRep and incrementing of referenceCount.

6.34.2.4 DakotaVarConstraints::~DakotaVarConstraints () `[virtual]`

destructor.

Destructor decrements referenceCount and only deletes varConstraintsRep when referenceCount reaches zero.

6.34.2.5 DakotaVarConstraints::DakotaVarConstraints (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 derived classes. get_var_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_var_constraints() again). Since the letter IS the representation, its rep pointer is set to NULL (an uninitialized pointer causes problems in ~DakotaVarConstraints).

6.34.3 Member Function Documentation

6.34.3.1 DakotaVarConstraints DakotaVarConstraints::operator= (const DakotaVarConstraints & *vc*)

assignment operator.

Assignment operator decrements referenceCount for old varConstraintsRep, assigns new varConstraints-Rep, and increments referenceCount for new varConstraintsRep.

6.34.3.2 void DakotaVarConstraints::manage_linear_constraints (const ProblemDescDB & *problem_db*, const size_t & *num_vars*) [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 passed up from the particular derived class.

6.34.3.3 DakotaVarConstraints * DakotaVarConstraints::get_var_constraints (const ProblemDescDB & *problem_db*) [private]

Used only by the constructor to initialize varConstraintsRep to the appropriate derived type.

Initializes varConstraintsRep to the appropriate derived type, as given by the variablesType attribute.

The documentation for this class was generated from the following files:

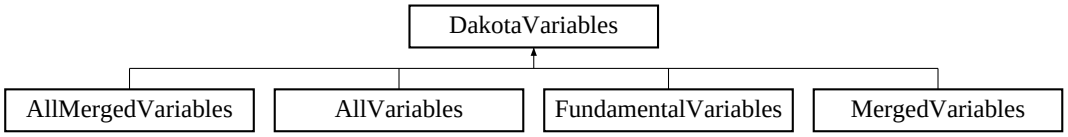
- DakotaVarConstraints.H
- DakotaVarConstraints.C

6.35 DakotaVariables Class Reference

Base class for the variables class hierarchy.

`#include <DakotaVariables.H>`

Inheritance diagram for DakotaVariables::



Public Methods

- DakotaVariables ()
  default constructor.
- DakotaVariables (const ProblemDescDB &problem_db)
  standard constructor.
- DakotaVariables (const DakotaString &vars_type)
  alternate constructor.
- DakotaVariables (const DakotaVariables &vars)
  copy constructor.
- virtual ~DakotaVariables ()
  destructor.
- DakotaVariables operator= (const DakotaVariables &vars)
  assignment operator.
- virtual size_t tv () const
  Returns total number of vars.
- virtual size_t cv () const
  Returns number of active continuous vars.
- virtual size_t dv () const
  Returns number of active discrete vars.
- virtual const DakotaRealVector & continuous_variables () const
  return the active continuous variables.
- virtual void continuous_variables (const DakotaRealVector &c_vars)

set the active continuous variables.

- virtual const DakotaIntVector & discrete_variables () const
  return the active discrete variables.
- virtual void discrete_variables (const DakotaIntVector &d_vars)
  set the active discrete variables.
- virtual const DakotaStringArray & continuous_variable_labels () const
  return the active continuous variable labels.
- virtual void continuous_variable_labels (const DakotaStringArray &cv_labels)
  set the active continuous variable labels.
- virtual const DakotaStringArray & discrete_variable_labels () const
  return the active discrete variable labels.
- virtual void discrete_variable_labels (const DakotaStringArray &dv_labels)
  set the active discrete variable labels.
- virtual const DakotaRealVector & inactive_continuous_variables () const
  return the inactive continuous variables.
- virtual void inactive_continuous_variables (const DakotaRealVector &i_c_vars)
  set the inactive continuous variables.
- virtual const DakotaIntVector & inactive_discrete_variables () const
  return the inactive discrete variables.
- virtual void inactive_discrete_variables (const DakotaIntVector &i_d_vars)
  set the inactive discrete variables.
- virtual size_t acv () const
  returns total number of continuous vars.
- virtual size_t adv () const
  returns total number of discrete vars.
- virtual DakotaRealVector all_continuous_variables () const
  returns a single array with all continuous variables.
- virtual DakotaIntVector all_discrete_variables () const
  returns a single array with all discrete variables.
- virtual void read (istream &s)
  read a variables object from an istream.
- virtual void write (ostream &s) const
  write a variables object to an ostream.

- virtual void read_annotated (istream &s)

  read a variables object in annotated format from an istream.

- virtual void write_annotated (ostream &s) const

  write a variables object in annotated format to an ostream.

- virtual void read (DakotaBiStream &s)

  read a variables object from the binary restart stream.

- virtual void write (DakotaBoStream &s) const

  write a variables object to the binary restart stream.

- virtual void read (UnPackBuffer &s)

  read a variables object from a packed MPI buffer.

- virtual void write (PackBuffer &s) const

  write a variables object to a packed MPI buffer.

- void write_tabular (ostream &s) const

  write a variables object in tabular format to an ostream.

- DakotaVariables copy () const

  for use when a true copy is needed (the representation is _not_ shared).

- const DakotaIntList & merged_integer_list () const

  returns the list of discrete variables merged into a continuous array.

- const DakotaString & variables_type () const

  returns the variables type: All, Merged, AllMerged, or Fundamental.

Protected Methods

- DakotaVariables (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).

Protected Attributes

- DakotaIntList mergedIntegerList

  the list of discrete variables for which integrality is relaxed by merging them into a continuous array.

- DakotaString variablesType

  All, Merged, AllMerged, or Fundamental.

- short apreproFlag

  used to trigger special behavior in write(ostream&).

Private Methods

- virtual void copy_rep (const DakotaVariables *vars_rep)

  Used by copy() to copy the contents of a letter class.

- DakotaVariables * get_variables (const ProblemDescDB &problem_db)

  Used by the standard envelope constructor to instantiate the correct letter class.

- DakotaVariables * get_variables (const DakotaString &vars_type) const

  Used by the alternate envelope constructor, by read functions, and by copy() to instantiate a new letter class.

Private Attributes

- DakotaVariables * variablesRep

  pointer to the letter (initialized only for the envelope).

- int referenceCount

  number of objects sharing variablesRep.

Friends

- int operator== (const DakotaVariables &vars1, const DakotaVariables &vars2)

  equality operator.

6.35.1 Detailed Description

Base class for the variables class hierarchy.

The DakotaVariables class is the base class for the class hierarchy providing design, uncertain, and state variables for continuous and discrete domains within a DakotaModel. 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 (DakotaVariables) serves as the envelope and one of the derived classes (selected in DakotaVariables::get_variables()) serves as the letter.

6.35.2 Constructor & Destructor Documentation

6.35.2.1 DakotaVariables::DakotaVariables ()

default constructor.

The default constructor: variablesRep is NULL in this case (a populated problem_db is needed to build a meaningful DakotaVariables object). This makes it necessary to check for NULL in the copy constructor, assignment operator, and destructor.

6.35.2.2 DakotaVariables::DakotaVariables (const ProblemDescDB & *problem_db*)

standard constructor.

This is the primary envelope constructor which uses problem_db to build a fully populated variables object. It only needs to extract enough data to properly execute get_variables(problem_db), since the constructor overloaded with BaseConstructor builds the actual base class data inherited by the derived classes.

6.35.2.3 DakotaVariables::DakotaVariables (const DakotaString & *vars_type*)

alternate constructor.

This is the alternate envelope constructor for instantiations on the fly. Since it does not have access to problem_db, the letter class is not fully populated. This constructor executes get_variables(vars_type), which invokes the default constructor of the derived letter class, which in turn invokes the default constructor of the base class.

6.35.2.4 DakotaVariables::DakotaVariables (const DakotaVariables & *vars*)

copy constructor.

Copy constructor manages sharing of variablesRep and incrementing of referenceCount.

6.35.2.5 DakotaVariables::~DakotaVariables () [virtual]

destructor.

Destructor decrements referenceCount and only deletes variablesRep when referenceCount reaches zero.

6.35.2.6 DakotaVariables::DakotaVariables (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 derived classes. get_variables() 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_variables() again). Since the letter IS the representation, its representation pointer is set to NULL (an uninitialized pointer causes problems in ~DakotaVariables).

6.35.3 Member Function Documentation

6.35.3.1 DakotaVariables DakotaVariables::operator= (const DakotaVariables & *vars*)

assignment operator.

Assignment operator decrements referenceCount for old variablesRep, assigns new variablesRep, and increments referenceCount for new variablesRep.

6.35.3.2 DakotaVariables DakotaVariables::copy () const

for use when a true copy is needed (the representation is _not_shared).

Deep copies are used for history mechanisms such as bestVariables and data_pairs since these must catalogue copies (and should not change as the representation within currentVariables changes).

6.35.3.3 DakotaVariables * DakotaVariables::get_variables (const ProblemDescDB & *problem_db*) [private]

Used by the standard envelope constructor to instantiate the correct letter class.

Initializes variablesRep to the appropriate derived type, as given by problem_db attributes. The standard derived class constructors are invoked.

6.35.3.4 DakotaVariables * DakotaVariables::get_variables (const DakotaString & *vars_type*) const [private]

Used by the alternate envelope constructor, by read functions, and by copy() to instantiate a new letter class.

Initializes variablesRep to the appropriate derived type, as given by the vars_type attribute. The default derived class constructors are invoked.

The documentation for this class was generated from the following files:

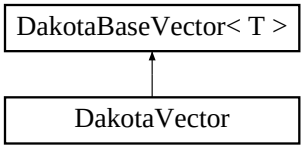
- DakotaVariables.H
- DakotaVariables.C

6.36 DakotaVector Class Template Reference

Template class for the Dakota numerical vector.

`#include <DakotaVector.H>`

Inheritance diagram for DakotaVector::



Public Methods

- DakotaVector ()
  Default constructor.
- DakotaVector (size_t size)
  Constructor which takes an initial size.
- DakotaVector (size_t size, const T &initial_val)
  Constructor which takes an initial size and an initial value.
- DakotaVector (const DakotaVector< T > &a)
  Copy constructor.
- DakotaVector (const T *p, size_t size)
  Constructor, creates array of size, with initial value <T> p.
- ~DakotaVector ()
  Destructor.
- void testClass ()
  Class unit test method.
- void read (istream &s)
  Reads a DakotaVector from an input stream.
- void read (istream &s, DakotaArray< DakotaString > &label_array)
  Reads a DakotaVector and associated label array from an input stream.
- void read_partial (istream &s, size_t start_index, size_t num_items)
  Reads part of a DakotaVector from an input stream.

- void read_partial (istream &s, size_t start_index, size_t num_items, DakotaArray< DakotaString > &label_array)

  Reads part of a DakotaVector and the corresponding labels from an input stream.

- void read_annotated (istream &s, DakotaArray< DakotaString > &label_array)

  Reads a DakotaVector and associated label array in annotated from an input stream.

- void print (ostream &s) const

  Prints a DakotaVector to an output stream.

- void print (ostream &s, const DakotaArray< DakotaString > &label_array) const

  Prints a DakotaVector and associated label array to an output stream.

- void print_partial (ostream &s, size_t start_index, size_t num_items) const

  Prints part of a DakotaVector to an output stream.

- void print_partial (ostream &s, size_t start_index, size_t num_items, const DakotaArray< DakotaString > &label_array) const

  Prints part of a DakotaVector and the corresponding labels to an output stream.

- void print_aprepro (ostream &s, const DakotaArray< DakotaString > &label_array) const

  Prints a DakotaVector and associated label array to an output stream in aprepro format.

- void print_partial_aprepro (ostream &s, size_t start_index, size_t num_items, const DakotaArray< DakotaString > &label_array) const

  Prints part of a DakotaVector and the corresponding labels to an output stream in aprepro format.

- void print_annotated (ostream &s, const DakotaArray< DakotaString > &label_array) const

  Prints a DakotaVector and associated label array in annotated form to an output stream.

- void read (DakotaBiStream &s, DakotaArray< DakotaString > &label_array)

  Reads a DakotaVector and associated label array from a binary input stream.

- void print (DakotaBoStream &s, const DakotaArray< DakotaString > &label_array) const

  Prints a DakotaVector and associated label array to a binary output stream.

- void read (UnPackBuffer &s)

  Reads a DakotaVector from a buffer after an MPI receive.

- void read (UnPackBuffer &s, DakotaArray< DakotaString > &label_array)

  Reads a DakotaVector and associated label array from a buffer after an MPI receive.

- void print (PackBuffer &s) const

  Writes a DakotaVector to a buffer prior to an MPI send.

- void print (PackBuffer &s, const DakotaArray< DakotaString > &label_array) const

  Writes a DakotaVector and associated label array to a buffer prior to an MPI send.

- DakotaVector< T > & operator= (const DakotaVector< T > &a)

  Normal const assignment operator.

- DakotaVector< T > & operator= (const T &ival)

  Sets all elements in self to the value ival.

- operator T * () const

  Converts the DakotaVector to a standard C-style array. Use with care!

Private Methods

- void copy_array (const T *p, size_t size)

  *Deep copies the array pointed to by {p} into this array. Private function for {operator=(const T *p)} and the constructor {DakotaVector(const T* p, size_t size)}.*

6.36.1 Detailed Description

template<class T> class DakotaVector< T >

Template class for the Dakota numerical vector.

The DakotaVector class is the numeric vector class . It inherits from the common vector class DakotaBase vector which provides the same interface for both the STL and RW vector classes. If the STL version of DakotaBaseVector is based on the valarray class then some basic vector operations such as + , * are available. This class adds functionallity to read/print vectors in a variety of ways

6.36.2 Constructor & Destructor Documentation

6.36.2.1 template<class T> DakotaVector< T >::DakotaVector (const T * *p*, size_t *size*)

Constructor, creates array of size, with initial value <T> p.

Assigns up to size values in array to p, uses the private copy_array method

6.36.3 Member Function Documentation

6.36.3.1 template<class T> void DakotaVector< T >::testClass ()

Class unit test method.

Unit test method for the DakotaVector class. Provides a quick way to test the basic functionallity of the class. Utilizes the assert function to test for correctness, will fail if an unexpected answer is received.

6.36.3.2 template<class T> DakotaVector< T > & DakotaVector< T >::operator= (const T & *ival*)

Sets all elements in self to the value ival.

Assigns all values of array to ival. If STL, uses the vector assign method because there is no operator=(ival).

Reimplemented from DakotaBaseVector.

6.36.3.3 template<class T> void DakotaVector< T >::copy_array (const T * *p*, size_t *size*) [private]

Deep copies the array pointed to by {p} into this array. Private function for {operator=(const T *p)} and the constructor {DakotaVector(const T* p, size_t size)}.

First resizes the vector to correct size and then assigns each value using the operator[ ](i).

The documentation for this class was generated from the following file:

- DakotaVector.H

6.37 DataInterface Class Reference

Container class for interface specification data.

`#include <DataInterface.H>`

Public Methods

- DataInterface ()

  constructor.

- DataInterface (const DataInterface &)

  copy constructor.

- ~DataInterface ()

  destructor.

- DataInterface & operator= (const DataInterface &)

  assignment operator.

- int operator== (const DataInterface &)

  equality operator.

- void write (ostream &s)

  write a DataInterface object to an ostream.

- void read (UnPackBuffer &s)

  read a DataInterface object from a packed MPI buffer.

- void write (PackBuffer &s)

  write a DataInterface object to a packed MPI buffer.

Public Attributes

- DakotaString interfaceType

  the interface selection: application_system/fork/direct/xml or approximation_ann/rsm/mars/hermite/ksm/mpa/taylor/hierarchical.

- DakotaString idInterface

  string identifier for an interface specification data set (from the id_interface specification in **InterfSetId***).*

- DakotaString inputFilter

  the input filter for a simulation-based interface (from the `input_filter` *specification in* **InterfApplic***).*

- DakotaString outputFilter

the output filter for a simulation-based interface (from the `output_filter` *specification in* **InterfApplic***).*

- DakotaStringList analysisDrivers

  the set of analysis drivers for a simulation-based interface (from the `analysis_drivers` *specification in* **InterfApplic***).*

- DakotaString parametersFile

  the parameters file for system call and fork interfaces (from the `parameters_file` *specification in* **InterfApplic***).*

- DakotaString resultsFile

  the results file for system call and fork interfaces (from the `results_file` *specification in* **InterfApplic***).*

- DakotaString analysisUsage

  the analysis command usage string for a system call interface (from the `analysis_usage` *specification in* **InterfApplic***).*

- short apreproFormatFlag

  the flag for aprepro format usage in the parameters file for system call and fork interfaces (from the `aprepro` *specification in* **InterfApplic***).*

- short fileTagFlag

  the flag for file tagging of parameters and results files for system call and fork interfaces (from the `file_tag` *specification in* **InterfApplic***).*

- short fileSaveFlag

  the flag for saving of parameters and results files for system call and fork interfaces (from the `file_save` *specification in* **InterfApplic***).*

- int procsPerAnalysis

  processors per parallel analysis for a direct interface (from the `processors_per_analysis` *specification in* **InterfApplic***).*

- DakotaStringList xmlHostNames

  names of host machines for an XML interface (from the `hostnames` *specification in* **InterfApplic***).*

- DakotaIntArray xmlProcsPerHost

  processors per host machine for an XML interface (from the `processors_per_host` *specification in* **InterfApplic***).*

- DakotaString interfaceSynchronization

  parallel mode for a simulation-based interface: synchronous or asynchronous (from the `asynchronous` *specification in* **InterfApplic***).*

- int asynchLocalEvalConcurrency

  evaluation concurrency for asynchronous simulation-based interfaces (from the `evaluation_concurrency` *specification in* **InterfApplic***).*

- int asynchLocalAnalysisConcurrency

  analysis concurrency for asynchronous simulation-based interfaces (from the `analysis_concurrency` *specification in* **InterfApplic***).*

- int evalServers

  number of evaluation servers to be used in the parallel configuration (from the `evaluation_servers` *specification in* **InterfApplic***).*

- DakotaString evalScheduling

  the scheduling approach to be used for concurrent evaluations within an iterator (from the `evaluation_self_scheduling` *and evaluation_static_scheduling specifications in* **InterfApplic***).*

- int analysisServers

  number of analysis servers to be used in the parallel configuration (from the `analysis_servers` *specification in* **InterfApplic***).*

- DakotaString analysisScheduling

  the scheduling approach to be used for concurrent analyses within a function evaluation (from the `analysis_self_scheduling` *and* `analysis_static_scheduling` *specifications in* **InterfApplic***).*

- DakotaString failAction

  the selected action upon capture of a simulation failure: abort, retry, recover, or continuation (from the `failure_capture` *specification in* **InterfApplic***).*

- int retryLimit

  the limit on retries for captured simulation failures (from the `retry` *specification in* **InterfApplic***).*

- DakotaRealVector recoveryFnVals

  the function values to be returned in a recovery operation for captured simulation failures (from the `recover` *specification in* **InterfApplic***).*

- short activeSetVectorFlag

  active set vector: 1=variable (ASV control on), 0=constant (ASV control off) (from the `active_set_vector` *specification in* **InterfApplic***).*

- DakotaString approxType

  the selected approximation type: global, multipoint, local, or hierarchical.

- DakotaString actualInterfacePtr

  pointer to the interface specification for constructing the truth model used in building local and multipoint approximations (from the `actual_interface_pointer` *specification in* **InterfApprox***).*

- DakotaString actualInterfaceResponsesPtr

  pointer to the responses specification for constructing the truth model used in building local approximations (from the `actual_interface_responses_pointer` *specification in* **InterfApprox***). This allows differences in gradient specifications between the responses used to build the approximation and the responses computed from the approximation.*

- DakotaString lowFidelityInterfacePtr

  pointer to the low fidelity interface specification used in hierarchical approximations (from the `low_fidelity_interface_pointer` *specification in* **InterfApprox***).*

- DakotaString highFidelityInterfacePtr

  pointer to the high fidelity interface specification used in hierarchical approximations (from the `high_fidelity_interface_pointer` *specification in* **InterfApprox***).*

- DakotaString approxDaceMethodPtr

  pointer to the design of experiments method used in building global approximations (from the `dace_method_pointer` *specification in* **InterfApprox***).*

- DakotaString approxSampleReuse

  sample reuse selection for building global approximations: none, all, or region (from the `reuse_samples` *specification in* **InterfApprox***).*

- DakotaString approxCorrection

  correction approach selection for global and hierarchical approximations: offset, scaled, or beta (from the `correction` *specification in* **InterfApprox***).*

- short approxGradUsageFlag

  flags the use of gradients in building global approximations (from the `use_gradients` *specification in* **InterfApprox***).*

- DakotaRealVector krigingCorrelations

  vector of correlations used in building a kriging approximation (from the `correlations` *specification in* **InterfApprox***).*

Private Methods

- void assign (const DataInterface &data_interface)

  convenience function for setting this objects attributes equal to the attributes of the incoming data_interface object (used by copy constructor and assignment operator).

6.37.1 Detailed Description

Container class for interface specification data.

The DataInterface class is used to contain the data from a interface keyword specification. It is populated by ProblemDescDB::interface_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataInterface objects is maintained in ProblemDescDB::interfaceList, one for each interface specification in an input file. Default values are managed in the DataInterface constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::interfaceList is private (a similar model is used with SurrogateDataPoint objects contained in DakotaApproximation and with ParallelismLevel objects contained in ParallelLibrary).

The documentation for this class was generated from the following files:

- DataInterface.H
- DataInterface.C

6.38 DataMethod Class Reference

Container class for method specification data.

`#include <DataMethod.H>`

Public Methods

- DataMethod ()
  constructor.
- DataMethod (const DataMethod &)
  copy constructor.
- ~DataMethod ()
  destructor.
- DataMethod & operator= (const DataMethod &)
  assignment operator.
- int operator== (const DataMethod &)
  equality operator.
- void write (ostream &s)
  write a DataMethod object to an ostream.
- void read (UnPackBuffer &s)
  read a DataMethod object from a packed MPI buffer.
- void write (PackBuffer &s)
  write a DataMethod object to a packed MPI buffer.

Public Attributes

- DakotaString methodName
  the method selection: one of the dot, npsol, opt++, apps, sgopt, nond, dace, or parameter study methods.
- DakotaString idMethod
  string identifier for the method specification data set (from the `id_method` *specification in* **MethodIndControl***).*
- DakotaString variablesPointer
  string pointer to the variables specification to be used by this method (from the `variables_pointer` *specification in* **MethodIndControl***).*
- DakotaString interfacePointer

string pointer to the interface specification to be used by this method (from the `interface_pointer` *specification in* **MethodIndControl***).*

- DakotaString responsesPointer

  string pointer to the responses specification to be used by this method (from the `responses_pointer` *specification in* **MethodIndControl***).*

- DakotaString modelType

  model type selection: single, nested, or layered (from the `model_type` *specification in* **MethodIndControl***).*

- DakotaString subMethodPointer

  string pointer to the sub-iterator used by nested models (from the `sub_method_pointer` *specification in* **MethodIndControl***).*

- DakotaString optionalInterfaceResponsesPointer

  string pointer to the responses specification used by the optional interface in nested models (from the `interface_responses_pointer` *specification in* **MethodIndControl***).*

- DakotaRealVector primaryCoeffs

  the primary mapping matrix used in nested models for weighting contributions from the sub-iterator responses in the top level (objective) functions (from the `primary_mapping_matrix` *specification in* **MethodIndControl***).*

- DakotaRealVector secondaryCoeffs

  the secondary mapping matrix used in nested models for weighting contributions from the sub-iterator responses in the top level (constraint) functions (from the `secondary_mapping_matrix` *specification in* **MethodIndControl***).*

- DakotaString methodOutput

  method verbosity control: quiet, verbose, debug, or normal (default) (from the `output` *specification in* **MethodIndControl***).*

- Real convergenceTolerance

  iteration convergence tolerance for the method (from the `convergence_tolerance` *specification in* **MethodIndControl***).*

- 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***).*

- int maxIterations

  maximum number of iterations allowed for the method (from the `max_iterations` *specification in* **MethodIndControl***).*

- int maxFunctionEvaluations

  maximum number of function evaluations allowed for the method (from the `max_function_evaluations` *specification in* **MethodIndControl***).*

- short 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***).*

- DakotaRealVector linearIneqConstraintCoeffs

  coefficient matrix for the linear inequality constraints (from the `linear_inequality_constraint_matrix` *specification in* **MethodIndControl***).*

- DakotaRealVector linearIneqLowerBnds

  lower bounds for the linear inequality constraints (from the `linear_inequality_lower_bounds` *specification in* **MethodIndControl***).*

- DakotaRealVector linearIneqUpperBnds

  upper bounds for the linear inequality constraints (from the `linear_inequality_upper_bounds` *specification in* **MethodIndControl***).*

- DakotaRealVector linearEqConstraintCoeffs

  coefficient matrix for the linear equality constraints (from the `linear_equality_constraint_matrix` *specification in* **MethodIndControl***).*

- DakotaRealVector linearEqTargets

  targets for the linear equality constraints (from the `linear_equality_targets` *specification in* **MethodIndControl***).*

- DakotaString daceMethod

  the dace method selection: grid, random, oas, lhs, oa_lhs, box_behnken_design, or central_composite_design (from the `dace` *specification in* **MethodDACE***).*

- DakotaString minMaxType

  the `optimization_type` *specification in* **MethodDOTDC**.

- int verifyLevel

  the `verify_level` *specification in* **MethodNPSOLDC**.

- Real functionPrecision

  the `function_precision` *specification in* **MethodNPSOLDC**.

- Real lineSearchTolerance

  the `linesearch_tolerance` *specification in* **MethodNPSOLDC**.

- DakotaString searchMethod

  the `search_method` *specification for Newton and NIPS methods in* **MethodOPTPPDC**.

- Real gradientTolerance

  the `gradient_tolerance` *specification in* **MethodOPTPPDC**.

- Real maxStep

  the `max_step` *specification in* **MethodOPTPPDC**.

- DakotaString meritFn

  the `merit_function` *specification for NIPS methods in* **MethodOPTPPDC**.

- DakotaString centralPath

  the `central_path` *specification for NIPS methods in* **MethodOPTPPDC**.

- Real stepLenToBoundary

  the `steplength_to_boundary` *specification for NIPS methods in* **MethodOPTPPDC**.

- Real centeringParam

  the `centering_parameter` *specification for NIPS methods in* **MethodOPTPPDC**.

- Real initialRadius

  the `initial_radius` *specification for ellipsoid methods in* **MethodOPTPPDC**.

- int searchSchemeSize

  the `search_scheme_size` *specification for PDS methods in* **MethodOPTPPDC**.

- Real solnAccuracy

  the `solution_accuracy` *specification in* **MethodSGOPTDC**.

- Real maxCPUTime

  the `max_cpu_time` *specification in* **MethodSGOPTDC**.

- Real crossoverRate

  the `crossover_rate` *specification for GA/EPSA methods in* **MethodSGOPTEA**.

- Real mutationDimRate

  the `dimension_rate` *specification for mutation in GA/EPSA methods in* **MethodSGOPTEA**.

- Real mutationPopRate

  the `population_rate` *specification for mutation in GA/EPSA methods in* **MethodSGOPTEA**.

- Real mutationScale

  the `mutation_scale` *specification for GA/EPSA methods in* **MethodSGOPTEA**.

- Real mutationMinScale

  the `min_scale` *specification for mutation in EPSA methods in* **MethodSGOPTEA**.

- Real initDelta

  the `initial_delta` *specification for APPS/PS/SW methods in* **MethodAPPSDC**, **MethodSGOPTPS**, *and* **MethodSGOPTSW**.

- Real threshDelta

  the `threshold_delta` *specification for APPS/PS/SW methods in* **MethodAPPSDC**, **MethodSGOPTPS**, *and* **MethodSGOPTSW**.

- Real contractFactor

  the `contraction_factor` *specification for APPS/PS/SW methods in* **MethodAPPSDC**, **MethodSGOPTPS**, *and* **MethodSGOPTSW**.

- int populationSize

  the `population_size` *specification for GA/EPSA methods in* **MethodSGOPTEA**.

- int newSolnsGenerated

the `new_solutions_generated` *specification for GA/EPSA methods in* **MethodSGOPTEA**.

- int numberRetained

  the integer assignment to random, chc, or elitist in the `replacement_type` *specification for GA/EPSA methods in* **MethodSGOPTEA**.

- int expandAfterSuccess

  the `expand_after_success` *specification for PS/SW methods in* **MethodSGOPTPS** *and* **MethodSGOPTSW**.

- int contractAfterFail

  the `contract_after_failure` *specification for the SW method in* **MethodSGOPTSW**.

- int mutationRange

  the `mutation_range` *specification for the pga_int method in* **MethodSGOPTEA**.

- int numPartitions

  the `num_partitions` *specification for EPSA methods in* **MethodSGOPTEA**.

- int totalPatternSize

  the `total_pattern_size` *specification for APPS/PS methods in* **MethodAPPSDC** *and* **MethodSGOPTPS**.

- int batchSize

  the `batch_size` *specification for the sMC method in* **MethodSGOPTSMC**.

- short nonAdaptiveFlag

  the `non_adaptive` *specification for the pga_real method in* **MethodSGOPTEA**.

- short randomizeOrderFlag

  the `stochastic` *specification for the PS method in* **MethodSGOPTPS**.

- short expansionFlag

  the `no_expansion` *specification for APPS/PS/SW methods in* **MethodAPPSDC**, **MethodSGOPTPS**, *and* **MethodSGOPTSW**.

- DakotaString selectionPressure

  the `selection_pressure` *specification for GA/EPSA methods in* **MethodSGOPTEA**.

- DakotaString replacementType

  the `replacement_type` *specification for GA/EPSA methods in* **MethodSGOPTEA**.

- DakotaString crossoverType

  the `crossover_type` *specification for GA/EPSA methods in* **MethodSGOPTEA**.

- DakotaString mutationType

  the `mutation_type` *specification for GA/EPSA methods in* **MethodSGOPTEA**.

- DakotaString exploratoryMoves

  the `exploratory_moves` *specification for the PS method in* **MethodSGOPTPS**.

- DakotaString patternBasis
  the `pattern_basis` *specification for APPS/PS methods in* **MethodAPPSDC** *and* **MethodSGOPTPS**.
- DakotaIntArray varPartitions
  the `partitions` *specification for sMC/PStudy methods in* **MethodSGOPTSMC** *and* **MethodPSMPS**.
- int randomSeed
  the `seed` *specification for SGOPT, NonD, & DACE methods.*
- int numSamples
  the `samples` *specification for NonD & DACE methods.*
- int numSymbols
  the `symbols` *specification for DACE methods.*
- int expansionTerms
  the `expansion_terms` *specification in* **MethodNonDPCE**.
- int expansionOrder
  the `expansion_order` *specification in* **MethodNonDPCE**.
- DakotaString sampleType
  the `sample_type` *specification in* **MethodNonDMC** *and* **MethodNonDPCE**.
- DakotaString reliabilityMethod
  the `amv/\c` *iterated_amv/*`form/\c` *sorm selection in* **MethodNonDAMV**.
- DakotaRealArray responseThresholds
  the `response_thresholds` *specification in* **MethodNonDMC** *and* **MethodNonDPCE**.
- DakotaRealArray responseLevels
  the `response_levels` *specification in* **MethodNonDAMV**.
- DakotaRealArray probabilityLevels
  the `probability_levels` *specification in* **MethodNonDAMV**.
- short allVarsFlag
  the `all_variables` *specification in* **MethodNonDMC**.
- int paramStudyType
  the type of parameter study: list(-1), vector(1, 2, or 3), centered(4), or multidim(5).
- DakotaRealVector finalPoint
  the `final_point` *specification in* **MethodPSVPS**.
- DakotaRealVector stepVector
  the `step_vector` *specification in* **MethodPSVPS**.
- Real stepLength
  the `step_length` *specification in* **MethodPSVPS**.

- int numSteps

  the `num_steps` *specification in* **MethodPSVPS**.

- DakotaRealVector listOfPoints

  the `list_of_points` *specification in* **MethodPSLPS**.

- Real percentDelta

  the `percent_delta` *specification in* **MethodPSCPS**.

- int deltasPerVariable

  the `deltas_per_variable` *specification in* **MethodPSCPS**.

Private Methods

- void assign (const DataMethod &data_method)

  convenience function for setting this objects attributes equal to the attributes of the incoming data_method object (used by copy constructor and assignment operator).

6.38.1 Detailed Description

Container class for method specification data.

The DataMethod class is used to contain the data from a method keyword specification. It is populated by ProblemDescDB::method_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataMethod objects is maintained in ProblemDescDB::methodList, one for each method specification in an input file. Default values are managed in the DataMethod constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::methodList is private (a similar model is used with SurrogateDataPoint objects contained in DakotaApproximation and with ParallelismLevel objects contained in ParallelLibrary).

The documentation for this class was generated from the following files:

- DataMethod.H
- DataMethod.C

6.39 DataResponses Class Reference

Container class for responses specification data.

`#include <DataResponses.H>`

Public Methods

- DataResponses ()
  constructor.
- DataResponses (const DataResponses &)
  copy constructor.
- ~DataResponses ()
  destructor.
- DataResponses & operator= (const DataResponses &)
  assignment operator.
- int operator== (const DataResponses &)
  equality operator.
- void write (ostream &s)
  write a DataResponses object to an ostream.
- void read (UnPackBuffer &s)
  read a DataResponses object from a packed MPI buffer.
- void write (PackBuffer &s)
  write a DataResponses object to a packed MPI buffer.

Public Attributes

- size_t numObjectiveFunctions
  number of objective functions (from the `num_objective_functions` *specification in* **RespFnOpt***).*
- 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 numLeastSquaresTerms

number of least squares terms (from the `num_least_squares_terms` *specification in* **RespFnLS***).*

- size_t numResponseFunctions

  number of generic response functions (from the `num_response_functions` *specification in* **RespFnGen***).*

- DakotaRealVector multiObjectiveWeights

  vector of multiobjective weightings (from the `multi_objective_weights` *specification in* **RespFnOpt***).*

- DakotaRealVector nonlinearIneqLowerBnds

  vector of nonlinear inequality constraint lower bounds (from the `nonlinear_inequality_lower_bounds` *specification in* **RespFnOpt***).*

- DakotaRealVector nonlinearIneqUpperBnds

  vector of nonlinear inequality constraint upper bounds (from the `nonlinear_inequality_upper_bounds` *specification in* **RespFnOpt***).*

- DakotaRealVector nonlinearEqTargets

  vector of nonlinear equality constraint targets (from the `nonlinear_equality_targets` *specification in* **RespFnOpt***).*

- DakotaString gradientType

  gradient type: none, numerical, analytic, or mixed (from the `no_gradients`, `numerical_gradients`, `analytic_gradients`, *and* `mixed_gradients` *specifications in* **RespGrad***).*

- DakotaString hessianType

  Hessian type: none or analytic (from the `no_hessians` *and* `analytic_hessians` *specifications in* **RespHess***).*

- DakotaString methodSource

  numerical gradient method source: dakota or vendor (from the `method_source` *specification in* **RespGradNum** *and* **RespGradMixed***).*

- DakotaString intervalType

  numerical gradient interval type: forward or central (from the `interval_type` *specification in* **RespGradNum** *and* **RespGradMixed***).*

- Real fdStepSize

  numerical gradient finite difference step size (from the `fd_step_size` *specification in* **RespGradNum** *and* **RespGradMixed***).*

- DakotaIntList idNumerical

  mixed gradient numerical identifiers (from the `id_numerical` *specification in* **RespGradMixed***).*

- DakotaIntList idAnalytic

  mixed gradient analytic identifiers (from the `id_analytic` *specification in* **RespGradMixed***).*

- DakotaString idResponses

  string identifier for the responses specification data set (from the `id_responses` *specification in* **RespSetId***).*

Private Methods

- void assign (const DataResponses &data_responses)

  convenience function for setting this objects attributes equal to the attributes of the incoming data_responses object (used by copy constructor and assignment operator).

6.39.1 Detailed Description

Container class for responses specification data.

The DataResponses class is used to contain the data from a responses keyword specification. It is populated by ProblemDescDB::responses_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataResponses objects is maintained in ProblemDescDB::responsesList, one for each responses specification in an input file. Default values are managed in the DataResponses constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::responsesList is private (a similar model is used with SurrogateDataPoint objects contained in DakotaApproximation and with ParallelismLevel objects contained in ParallelLibrary).

The documentation for this class was generated from the following files:

- DataResponses.H
- DataResponses.C

6.40 DataVariables Class Reference

Container class for variables specification data.

`#include <DataVariables.H>`

Public Methods

- DataVariables ()
  constructor.
- DataVariables (const DataVariables &)
  copy constructor.
- ~DataVariables ()
  destructor.
- DataVariables & operator= (const DataVariables &)
  assignment operator.
- int operator== (const DataVariables &)
  equality operator.
- void write (ostream &s)
  write a DataVariables object to an ostream.
- void read (UnPackBuffer &s)
  read a DataVariables object from a packed MPI buffer.
- void write (PackBuffer &s)
  write a DataVariables object to a packed MPI buffer.
- size_t design ()
  return total number of design variables.
- size_t uncertain ()
  return total number of uncertain variables.
- size_t state ()
  return total number of state variables.
- size_t num_continuous_variables ()
  return total number of continuous variables.
- size_t num_discrete_variables ()
  return total number of discrete variables.

- size_t num_variables ()

  return total number of variables.

Public Attributes

- DakotaString idVariables

  string identifier for the variables specification data set (from the `id_variables` *specification in* **VarSet-Id***).*

- size_t numContinuousDesVars

  number of continuous design variables (from the `continuous_design` *specification in* **VarDV***).*

- size_t numDiscreteDesVars

  number of discrete design variables (from the `discrete_design` *specification in* **VarDV***).*

- size_t numNormalUncVars

  number of normal uncertain variables (from the `normal_uncertain` *specification in* **VarUV***).*

- size_t numLognormalUncVars

  number of lognormal uncertain variables (from the `lognormal_uncertain` *specification in* **VarUV***).*

- size_t numUniformUncVars

  number of uniform uncertain variables (from the `uniform_uncertain` *specification in* **VarUV***).*

- size_t numLoguniformUncVars

  number of loguniform uncertain variables (from the `loguniform_uncertain` *specification in* **VarUV***).*

- size_t numWeibullUncVars

  number of weibull uncertain variables (from the `weibull_uncertain` *specification in* **VarUV***).*

- size_t numHistogramUncVars

  number of histogram uncertain variables (from the `histogram_uncertain` *specification in* **VarUV***).*

- size_t numContinuousStateVars

  number of continuous state variables (from the `continuous_state` *specification in* **VarSV***).*

- size_t numDiscreteStateVars

  number of discrete state variables (from the `discrete_state` *specification in* **VarSV***).*

- DakotaRealVector continuousDesignVars

  initial values for the continuous design variables array (from the `cdv_initial_point` *specification in* **VarDV***).*

- DakotaRealVector continuousDesignLowerBnds

  the continuous design lower bounds array (from the `cdv_lower_bounds` *specification in* **VarDV***).*

- DakotaRealVector continuousDesignUpperBnds

  the continuous design upper bounds array (from the `cdv_upper_bounds` *specification in* **VarDV***).*

- DakotaIntVector discreteDesignVars

  initial values for the discrete design variables array (from the `ddv_initial_point` *specification in* **VarDV***).*

- DakotaIntVector discreteDesignLowerBnds

  the discrete design lower bounds array (from the `ddv_lower_bounds` *specification in* **VarDV***).*

- DakotaIntVector discreteDesignUpperBnds

  the discrete design upper bounds array (from the `ddv_upper_bounds` *specification in* **VarDV***).*

- DakotaStringArray continuousDesignLabels

  the continuous design labels array (from the `cdv_descriptor` *specification in* **VarDV***).*

- DakotaStringArray discreteDesignLabels

  the discrete design labels array (from the `ddv_descriptor` *specification in* **VarDV***).*

- DakotaRealVector normalUncMeans

  means of the normal uncertain variables (from the `nuv_means` *specification in* **VarUV***).*

- DakotaRealVector normalUncStdDevs

  standard deviations of the normal uncertain variables (from the `nuv_std_deviations` *specification in* **VarUV***).*

- DakotaRealVector normalUncDistLowerBnds

  distribution lower bounds for the normal uncertain variables (from the `nuv_dist_lower_bounds` *specification in* **VarUV***).*

- DakotaRealVector normalUncDistUpperBnds

  distribution upper bounds for the normal uncertain variables (from the `nuv_dist_upper_bounds` *specification in* **VarUV***).*

- DakotaRealVector lognormalUncMeans

  means of the lognormal uncertain variables (from the `lnuv_means` *specification in* **VarUV***).*

- DakotaRealVector lognormalUncStdDevs

  standard deviations of the lognormal uncertain variables (from the `lnuv_std_deviations` *specification in* **VarUV***).*

- DakotaRealVector lognormalUncErrFacts

  error factors for the lognormal uncertain variables (from the `lnuv_error_factors` *specification in* **VarUV***).*

- DakotaRealVector lognormalUncDistLowerBnds

  distribution lower bounds for the lognormal uncertain variables (from the `lnuv_dist_lower_bounds` *specification in* **VarUV***).*

- DakotaRealVector lognormalUncDistUpperBnds

  distribution upper bounds for the lognormal uncertain variables (from the `lnuv_dist_upper_bounds` *specification in* **VarUV***).*

- DakotaRealVector uniformUncDistLowerBnds

distribution lower bounds for the uniform uncertain variables (from the `uuv_dist_lower_bounds` *specification in* **VarUV***).*

- DakotaRealVector uniformUncDistUpperBnds

  distribution upper bounds for the uniform uncertain variables (from the `uuv_dist_upper_bounds` *specification in* **VarUV***).*

- DakotaRealVector loguniformUncDistLowerBnds

  distribution lower bounds for the loguniform uncertain variables (from the `luuv_dist_lower_bounds` *specification in* **VarUV***).*

- DakotaRealVector loguniformUncDistUpperBnds

  distribution upper bounds for the loguniform uncertain variables (from the `luuv_dist_upper_bounds` *specification in* **VarUV***).*

- DakotaRealVector weibullUncAlphas

  alpha factors for the weibull uncertain variables (from the `wuv_alphas` *specification in* **VarUV***).*

- DakotaRealVector weibullUncBetas

  beta factors for the weibull uncertain variables (from the `wuv_betas` *specification in* **VarUV***).*

- DakotaRealVector weibullUncDistLowerBnds

  distribution lower bounds for the weibull uncertain variables (from the `wuv_dist_lower_bounds` *specification in* **VarUV***).*

- DakotaRealVector weibullUncDistUpperBnds

  distribution upper bounds for the weibull uncertain variables (from the `wuv_dist_upper_bounds` *specification in* **VarUV***).*

- DakotaRealVector histogramUncDistLowerBnds

  distribution lower bounds for the histogram uncertain variables (from the `huv_dist_lower_bounds` *specification in* **VarUV***).*

- DakotaRealVector histogramUncDistUpperBnds

  distribution upper bounds for the histogram uncertain variables (from the `huv_dist_upper_bounds` *specification in* **VarUV***).*

- DakotaStringList histogramUncFilenames

  filenames containing the histograms for the histogram uncertain variables (from the `huv_filenames` *specification in* **VarUV***).*

- DakotaRealMatrix uncertainCorrelations

  correlation matrix for all uncertain variables (from the `uncertain_correlation_matrix` *specification in* **VarUV***). This matrix specifies rank correlations for sampling methods (i.e., LHS) and correlation coefficients (rho_ij = normalized covariance matrix) for analytic reliability methods.*

- DakotaRealVector uncertainVars

  array of values for all uncertain variables (built and initialized in ProblemDescDB::variables_kwhandler()).

- DakotaRealVector uncertainDistLowerBnds

distribution lower bounds for all uncertain variables (collected from `nuv_dist_lower_bounds`, `lnuv_dist_lower_bounds`, `uuv_dist_lower_bounds`, `luuv_dist_lower_bounds`, `wuv_dist_lower_bounds`, *and* `huv_dist_lower_bounds` *specifications in* **VarUV***).*

- DakotaRealVector uncertainDistUpperBnds

  distribution upper bounds for all uncertain variables (collected from `nuv_dist_upper_bounds`, `lnuv_dist_upper_bounds`, `uuv_dist_upper_bounds`, `luuv_dist_upper_bounds`, `wuv_dist_upper_bounds`, *and* `huv_dist_upper_bounds` *specifications in* **VarUV***).*

- DakotaStringArray uncertainLabels

  labels for all uncertain variables (collected from `nuv_descriptor`, `lnuv_descriptor`, `uuv_descriptor`, `luuv_descriptor`, `wuv_descriptor`, *and* `huv_descriptor` *specifications in* **VarUV***).*

- DakotaRealVector continuousStateVars

  initial values for the continuous state variables array (from the `csv_initial_state` *specification in* **VarSV***).*

- DakotaRealVector continuousStateLowerBnds

  the continuous state lower bounds array (from the `csv_lower_bounds` *specification in* **VarSV***).*

- DakotaRealVector continuousStateUpperBnds

  the continuous state upper bounds array (from the `csv_upper_bounds` *specification in* **VarSV***).*

- DakotaIntVector discreteStateVars

  initial values for the discrete state variables array (from the `dsv_initial_state` *specification in* **VarSV***).*

- DakotaIntVector discreteStateLowerBnds

  the discrete state lower bounds array (from the `dsv_lower_bounds` *specification in* **VarSV***).*

- DakotaIntVector discreteStateUpperBnds

  the discrete state upper bounds array (from the `dsv_upper_bounds` *specification in* **VarSV***).*

- DakotaStringArray continuousStateLabels

  the continuous state labels array (from the `csv_descriptor` *specification in* **VarSV***).*

- DakotaStringArray discreteStateLabels

  the discrete state labels array (from the `dsv_descriptor` *specification in* **VarSV***).*

Private Methods

- void assign (const DataVariables &data_variables)

  convenience function for setting this objects attributes equal to the attributes of the incoming data_variables object (used by copy constructor and assignment operator).

6.40.1 Detailed Description

Container class for variables specification data.

The DataVariables class is used to contain the data from a variables keyword specification. It is populated by ProblemDescDB::variables_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. A list of DataVariables objects is maintained in ProblemDescDB::variablesList, one for each variables specification in an input file. Default values are managed in the DataVariables constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::variablesList is private (a similar model is used with SurrogateDataPoint objects contained in DakotaApproximation and with ParallelismLevel objects contained in ParallelLibrary).

The documentation for this class was generated from the following files:

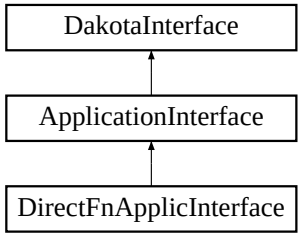
- DataVariables.H
- DataVariables.C

6.41 DirectFnApplicInterface Class Reference

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

`#include <DirectFnApplicInterface.H>`

Inheritance diagram for DirectFnApplicInterface::



Public Methods

- DirectFnApplicInterface (const ProblemDescDB &problem_db, const size_t &num_fns)

  constructor.

- ~DirectFnApplicInterface ()

  destructor.

- void derived_map (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &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 derived_synch (DakotaList< ParamResponsePair > &prp_list)

  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 derived_synch_nowait (DakotaList< ParamResponsePair > &prp_list)

  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 derived_synchronous_local_analysis (const 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().

Private Methods

- int derived_map_if (const DakotaString &if_name)

  execute the input filter portion of a direct evaluation invocation.

- int derived_map_ac (const DakotaString &ac_name)

  execute an analysis code portion of a direct evaluation invocation.

- int derived_map_of (const DakotaString &of_name)

  execute the output filter portion of a direct evaluation invocation.

- void set_local_data ()

  convenience function for local test simulators which sets variable attributes and zeros response data.

- void overlay_response (DakotaResponse &response)

  convenience function for local test simulators which overlays response contributions from multiple analyses using MPI_Reduce.

- int cyl_head (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  the cylinder head constrained optimization test function.

- int rosenbrock (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  the rosenbrock optimization and least squares test function.

- int text_book (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  the text_book constrained optimization test function.

- int text_book1 (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  portion of text_book() evaluating the objective function and its derivatives.

- int text_book2 (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  portion of text_book() evaluating constraint 1 and its derivatives.

- int text_book3 (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  portion of text_book() evaluating constraint 2 and its derivatives.

- int salinas (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  direct interface to the SALINAS structural dynamics simulation code.

Private Attributes

- DakotaString iFilterName

  name of the direct function input filter.

- DakotaString oFilterName

  name of the direct function output filter.

- short gradFlag

  signals use of fnGrads in direct simulator functions.

- short 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 numGradVars

  number of continuous variables.

- DakotaRealVector xVect

  continuous and discrete variable set used within direct simulator functions.

- DakotaRealVector fnVals

  response function values set within direct simulator functions.

- DakotaRealMatrix fnGrads

  response function gradients set within direct simulator functions.

- DakotaRealMatrixArray fnHessians

  response function Hessians set within direct simulator functions.

- DakotaVariables directFnVars

  class scope variables object.

- DakotaIntArray directFnASV

  class scope active set vector object.

- DakotaResponse directFnResponse

  class scope response object.

6.41.1 Detailed Description

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

DerivedFnApplicInterface uses a few linkable simulation codes and several internal member functions to perform parameter to response mappings.

The documentation for this class was generated from the following files:

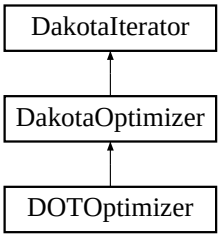
- DirectFnApplicInterface.H
- DirectFnApplicInterface.C

6.42 DOTOptimizer Class Reference

Wrapper class for the DOT optimization library.

`#include <DOTOptimizer.H>`

Inheritance diagram for DOTOptimizer::



Public Methods

- DOTOptimizer (DakotaModel &model)

  constructor.

- ~DOTOptimizer ()

  destructor.

- void find_optimum ()

  Used within the optimizer branch for computing the optimal solution. Redefines the run_iterator virtual function for the optimizer branch.

Private Methods

- void allocate_workspace ()

  Allocates workspace for the optimizer.

Private Attributes

- int dotInfo

  INFO from DOT manual.

- int dotFDSinfo

  internal DOT parameter NGOTOZ.

- int dotMethod

  METHOD from DOT manual.

- int printControl

  IPRINT from DOT manual (controls output verbosity).

- int optimizationType

  MINMAX from DOT manual (minimize or maximize).

- DakotaRealArray realCntlParmArray

  RPRM from DOT manual.

- DakotaIntArray intCntlParmArray

  IPRM from DOT manual.

- DakotaRealVector localConstraintValues

  array of nonlinear constraint values passed to DOT.

- DakotaSizetList constraintMappingIndices

  a list of indices for referencing the corresponding DakotaResponse constraints used in computing the DOT constraints.

- DakotaRealList constraintMappingMultipliers

  a list of multipliers for mapping the DakotaResponse constraints to the DOT constraints.

- DakotaRealList constraintMappingOffsets

  a list of offsets for mapping the DakotaResponse constraints to the DOT constraints.

6.42.1 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 function and static attribute 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 find_optimum() 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.

6.42.2 Member Data Documentation

6.42.2.1 int DOTOptimizer::dotInfo [private]

INFO from DOT manual.

Information requested by DOT: 0=optimization complete, 1=get values, 2=get gradients

6.42.2.2 int DOTOptimizer::dotFDSinfo [private]

internal DOT parameter NGOTOZ.

the DOT parameter list has been modified to pass NGOTOZ, which signals whether DOT is finite-differencing (nonzero value) or performing the line search (zero value).

6.42.2.3 int DOTOptimizer::dotMethod [private]

METHOD from DOT manual.

For nonlinear constraints: 0/1 = dot_mmfd, 2 = dot_slp, 3 = dot_sqp. For unconstrained: 0/1 = dot_bfgs, 2 = dot_frcg.

6.42.2.4 int DOTOptimizer::printControl [private]

IPRINT from DOT manual (controls output verbosity).

Values range from 0 (least output) to 7 (most output).

6.42.2.5 int DOTOptimizer::optimizationType [private]

MINMAX from DOT manual (minimize or maximize).

Values of 0 or -1 (minimize) or 1 (maximize).

6.42.2.6 DakotaRealArray DOTOptimizer::realCntlParmArray [private]

RPRM from DOT manual.

Array of real control parameters.

6.42.2.7 DakotaIntArray DOTOptimizer::intCntlParmArray [private]

IPRM from DOT manual.

Array of integer control parameters.

6.42.2.8 DakotaRealVector DOTOptimizer::localConstraintValues [private]

array of nonlinear constraint values passed to DOT.

This array must be of nonzero length (sized with localConstraintArraySize) and must contain only one-sided inequality constraints which are <= 0 (which requires a transformation from 2-sided inequalities and equalities).

6.42.2.9 DakotaSizetList DOTOptimizer::constraintMappingIndices [private]

a list of indices for referencing the corresponding DakotaResponse constraints used in computing the DOT constraints.

The length of the list corresponds to the number of DOT constraints, and each entry in the list points to the corresponding DAKOTA constraint.

6.42.2.10 DakotaRealList DOTOptimizer::constraintMappingMultipliers [private]

a list of multipliers for mapping the DakotaResponse constraints to the DOT constraints.

The length of the list corresponds to the number of DOT constraints, and each entry in the list contains a multiplier for the DAKOTA constraint identified with constraintMappingIndices. These multipliers are currently +1 or -1.

6.42.2.11 DakotaRealList DOTOptimizer::constraintMappingOffsets [private]

a list of offsets for mapping the DakotaResponse constraints to the DOT constraints.

The length of the list corresponds to the number of DOT constraints, and each entry in the list contains an offset for the DAKOTA constraint identified with constraintMappingIndices. These offsets involve inequality bounds or equality targets, since DOT assumes constraint allowables = 0.

The documentation for this class was generated from the following files:

- DOTOptimizer.H
- DOTOptimizer.C

6.43 ErrorTable Struct Reference

Data structure to hold errors.

Public Attributes

- CtelRegexp::RStatus rc

  Enumerated type to hold status codes.

- const char * msg

  Holds character string error message.

6.43.1 Detailed Description

Data structure to hold errors.

This module implements a C++ wrapper for Regular Expressions based on the public domain engine for regular expressions released by: Copyright (c) 1986 by University of Toronto. Written by Henry Spencer. Not derived from licensed software.

The documentation for this struct was generated from the following file:

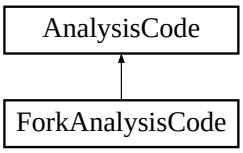
- CtelRegExp.C

6.44 ForkAnalysisCode Class Reference

Derived class in the AnalysisCode class hierarchy which spawns simulations using forks.

`#include <ForkAnalysisCode.H>`

Inheritance diagram for ForkAnalysisCode::



Public Methods

- ForkAnalysisCode (const ProblemDescDB &problem_db)

  constructor.

- ~ForkAnalysisCode ()

  destructor.

- pid_t fork_program (const short block_flag)

  spawn a child process using fork()/vfork()/execvp() and wait for completion using waitpid() if block_flag is true.

- void check_status (const int status)

  check the exit status of a forked process and abort if an error code was returned.

- void argument_list (const int index, const DakotaString &arg)

  set argList[index] to arg.

- void tag_argument_list (const int index, const int tag)

  append an additional tag to argList[index] (beyond that already present in the modified file names) for managing concurrent analyses within a function evaluation.

Private Attributes

- const char * argList [4]

  *an array of strings for use with execvp(const char *, char * const *) (an argList entry can be passed as the first argument, and the entire argList can be cast as the second argument).*

6.44.1 Detailed Description

Derived class in the AnalysisCode class hierarchy which spawns simulations using forks.

ForkAnalysisCode creates a copy of the parent DAKOTA process using fork()/vfork() and then replaces the copy with a simulation process using execvp(). The parent process can then use waitpid() to wait on completion of the simulation process.

6.44.2 Member Function Documentation

6.44.2.1 void ForkAnalysisCode::check_status (const int *status*)

check the exit status of a forked process and abort if an error code was returned.

Check to see if the 3-piece interface 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().

The documentation for this class was generated from the following files:

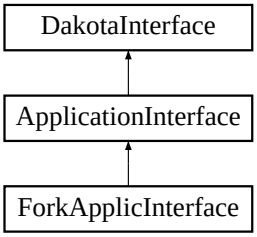
- ForkAnalysisCode.H
- ForkAnalysisCode.C

6.45 ForkApplicInterface Class Reference

Derived application interface class which spawns simulation codes using forks.

`#include <ForkApplicInterface.H>`

Inheritance diagram for ForkApplicInterface::



Public Methods

- ForkApplicInterface (const ProblemDescDB &problem_db, const size_t &num_fns)

  constructor.

- ~ForkApplicInterface ()

  destructor.

- void derived_map (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &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 derived_synch (DakotaList< ParamResponsePair > &prp_list)

  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 derived_synch_nowait (DakotaList< ParamResponsePair > &prp_list)

  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 derived_synchronous_local_analysis (const 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().

Private Methods

- void derived_synch_kernel (DakotaList< ParamResponsePair > &prp_list, const pid_t pid)

  Convenience function for common code between derived_synch() & derived_synch_nowait().

- pid_t fork_application (const short block_flag)

  perform the complete function evaluation by managing the input filter, analysis programs, and output filter.

- void asynchronous_local_analyses (const int &start, const int &end, const int &step)

  execute analyses asynchronously on the local processor.

- void synchronous_local_analyses (const int &start, const int &end, const int &step)

  execute analyses synchronously on the local processor.

- void serve_analyses_asynch ()

  serve the analysis scheduler and execute analysis assignments asynchronously.

Private Attributes

- ForkAnalysisCode forkSimulator

  ForkAnalysisCode provides convenience functions for forking individual programs and checking fork exit status.

- DakotaList< pid_t > processIdList

  list of process id's for asynchronous evaluations; correspondence to evalIdList used for mapping captured fork process id's to function evaluation id's.

- DakotaIntList evalIdList

  list of function evaluation id's for asynchronous evaluations; correspondence to processIdList used for mapping captured fork process id's to function evaluation id's.

6.45.1 Detailed Description

Derived application interface class which spawns simulation codes using forks.

ForkApplicInterface uses a ForkAnalysisCode object for performing simulation invocations.

6.45.2 Member Function Documentation

6.45.2.1 pid_t ForkApplicInterface::fork_application (const short *block_flag*) [private]

perform the complete function evaluation by managing the input filter, analysis programs, and output filter.

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 ForkAnalysisCode::fork_program() to spawn individual program components within the function evaluation.

6.45.2.2 void ForkApplicInterface::asynchronous_local_analyses (const int & *start*, const int & *end*, const int & *step*) [private]

execute analyses asynchronously on the local processor.

Schedule analyses asynchronously on the local processor using a self-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.

6.45.2.3 void ForkApplicInterface::synchronous_local_analyses (const int & *start*, const int & *end*, const int & *step*) [private]

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().

6.45.2.4 void ForkApplicInterface::serve_analyses_asynch () [private]

serve the analysis scheduler and execute analysis assignments 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.

The documentation for this class was generated from the following files:

- ForkApplicInterface.H
- ForkApplicInterface.C

6.46 FunctionCompare Class Template Reference

`#include <DakotaList.H>`

Public Methods

- FunctionCompare (int(∗func)(const T &, void ∗), void ∗v)

  Constructor that defines the pointer to function and search value.

- bool operator() (T t) const

  The operator() must be defined. Calls the function testFunction.

Private Attributes

- int(∗ testFunction)(const T &, void ∗)

  Pointer to test function.

- void ∗ search_val

  Holds the value to search for.

6.46.1 Detailed Description

template<class T> class FunctionCompare< T >

Internal Functor to mimick the RW find and index functions using the STL find_if() method. The class holds a pointer to the test function and the search value.

The documentation for this class was generated from the following file:

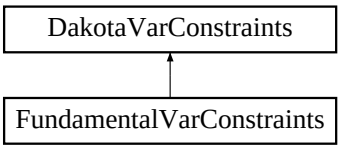
- DakotaList.H

6.47 FundamentalVarConstraints Class Reference

Derived class within the DakotaVarConstraints hierarchy which employs the default data view (no variable or domain type array merging).

`#include <FundamentalVarConstraints.H>`

Inheritance diagram for FundamentalVarConstraints::



Public Methods

- FundamentalVarConstraints (const ProblemDescDB &problem_db)
  constructor.
- ~FundamentalVarConstraints ()
  destructor.
- const DakotaRealVector & continuous_lower_bounds () const
  return the active continuous variable lower bounds.
- void continuous_lower_bounds (const DakotaRealVector &c_l_bnds)
  set the active continuous variable lower bounds.
- const DakotaRealVector & continuous_upper_bounds () const
  return the active continuous variable upper bounds.
- void continuous_upper_bounds (const DakotaRealVector &c_u_bnds)
  set the active continuous variable upper bounds.
- const DakotaIntVector & discrete_lower_bounds () const
  return the active discrete variable lower bounds.
- void discrete_lower_bounds (const DakotaIntVector &d_l_bnds)
  set the active discrete variable lower bounds.
- const DakotaIntVector & discrete_upper_bounds () const
  return the active discrete variable upper bounds.
- void discrete_upper_bounds (const DakotaIntVector &d_u_bnds)
  set the active discrete variable upper bounds.

- void write (ostream &s) const

  write a variable constraints object to an ostream.

- void read (istream &s)

  read a variable constraints object from an istream.

Private Attributes

- short nonDFlag

  this flag is set if uncertain variables are active (the default is design variables are active; see constructor for logic).

- DakotaRealVector continuousDesignLowerBnds

  the continuous design lower bounds array.

- DakotaRealVector continuousDesignUpperBnds

  the continuous design upper bounds array.

- DakotaIntVector discreteDesignLowerBnds

  the discrete design lower bounds array.

- DakotaIntVector discreteDesignUpperBnds

  the discrete design upper bounds array.

- DakotaRealVector uncertainDistLowerBnds

  the uncertain distribution lower bounds array.

- DakotaRealVector uncertainDistUpperBnds

  the uncertain distribution upper bounds array.

- DakotaRealVector continuousStateLowerBnds

  the continuous state lower bounds array.

- DakotaRealVector continuousStateUpperBnds

  the continuous state upper bounds array.

- DakotaIntVector discreteStateLowerBnds

  the discrete state lower bounds array.

- DakotaIntVector discreteStateUpperBnds

  the discrete state upper bounds array.

- DakotaRealVector emptyRealVector

  an empty real vector returned in get functions when there are no variables corresponding to the request.

- DakotaIntVector emptyIntVector

  an empty int vector returned in get functions when there are no variables corresponding to the request.

6.47.1 Detailed Description

Derived class within the DakotaVarConstraints hierarchy which employs the default data view (no variable or 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 FundamentalVarConstraints derived class separates the design, uncertain, and state variable types as well as the continuous and discrete domain types. The result is separate lower and upper bounds arrays for continuous design, discrete design, uncertain, continuous state, and discrete state variables. This is the default approach, so all iterators and strategies not specifically utilizing the All, Merged, or AllMerged views use this approach (see DakotaVariables::get_variables(problem_db) for variables type selection; variables type is passed to the DakotaVarConstraints constructor in DakotaModel).

6.47.2 Constructor & Destructor Documentation

6.47.2.1 FundamentalVarConstraints::FundamentalVarConstraints (const ProblemDescDB & *problem_db*)

constructor.

Extract fundamental lower and upper bounds (VariablesUtil is not used).

The documentation for this class was generated from the following files:

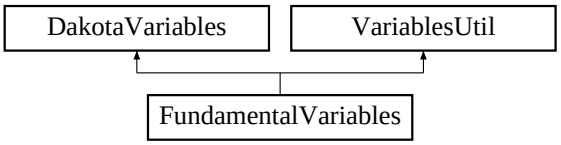
- FundamentalVarConstraints.H
- FundamentalVarConstraints.C

6.48 FundamentalVariables Class Reference

Derived class within the DakotaVariables hierarchy which employs the default data view (no variable or domain type array merging).

`#include <FundamentalVariables.H>`

Inheritance diagram for FundamentalVariables::



Public Methods

- FundamentalVariables ()
  default constructor.
- FundamentalVariables (const ProblemDescDB &problem_db)
  standard constructor.
- ~FundamentalVariables ()
  destructor.
- size_t tv () const
  Returns total number of vars.
- size_t cv () const
  Returns number of active continuous vars.
- size_t dv () const
  Returns number of active discrete vars.
- const DakotaRealVector & continuous_variables () const
  return the active continuous variables.
- void continuous_variables (const DakotaRealVector &c_vars)
  set the active continuous variables.
- const DakotaIntVector & discrete_variables () const
  return the active discrete variables.
- void discrete_variables (const DakotaIntVector &d_vars)
  set the active discrete variables.

- const DakotaStringArray & continuous_variable_labels () const
  return the active continuous variable labels.
- void continuous_variable_labels (const DakotaStringArray &cv_labels)
  set the active continuous variable labels.
- const DakotaStringArray & discrete_variable_labels () const
  return the active discrete variable labels.
- void discrete_variable_labels (const DakotaStringArray &dv_labels)
  set the active discrete variable labels.
- const DakotaRealVector & inactive_continuous_variables () const
  return the inactive continuous variables.
- void inactive_continuous_variables (const DakotaRealVector &i_c_vars)
  set the inactive continuous variables.
- const DakotaIntVector & inactive_discrete_variables () const
  return the inactive discrete variables.
- void inactive_discrete_variables (const DakotaIntVector &i_d_vars)
  set the inactive discrete variables.
- size_t acv () const
  returns total number of continuous vars.
- size_t adv () const
  returns total number of discrete vars.
- DakotaRealVector all_continuous_variables () const
  returns a single array with all continuous variables.
- DakotaIntVector all_discrete_variables () const
  returns a single array with all discrete variables.
- void read (istream &s)
  read a variables object from an istream.
- void write (ostream &s) const
  write a variables object to an ostream.
- void read_annotated (istream &s)
  read a variables object in annotated format from an istream.
- void write_annotated (ostream &s) const
  write a variables object in annotated format to an ostream.
- void read (DakotaBiStream &s)
  read a variables object from the binary restart stream.

- void write (DakotaBoStream &s) const

  write a variables object to the binary restart stream.

- void read (UnPackBuffer &s)

  read a variables object from a packed MPI buffer.

- void write (PackBuffer &s) const

  write a variables object to a packed MPI buffer.

Private Methods

- void copy_rep (const DakotaVariables *vars_rep)

  Used by copy() to copy the contents of a letter class.

Private Attributes

- short nonDFlag

  this flag is set if uncertain variables are active (the default is design variables are active; see constructor for logic).

- DakotaRealVector continuousDesignVars

  the continuous design variables array.

- DakotaIntVector discreteDesignVars

  the discrete design variables array.

- DakotaRealVector uncertainVars

  the uncertain variables array.

- DakotaRealVector continuousStateVars

  the continuous state variables array.

- DakotaIntVector discreteStateVars

  the discrete state variables array.

- DakotaStringArray continuousDesignLabels

  the continuous design variables label array.

- DakotaStringArray discreteDesignLabels

  the discrete design variables label array.

- DakotaStringArray uncertainLabels

  the uncertain variables label array.

- DakotaStringArray continuousStateLabels

  the continuous state variables label array.

- DakotaStringArray discreteStateLabels
  the discrete state variables label array.
- DakotaRealVector emptyRealVector
  an empty real vector returned in get functions when there are no variables corresponding to the request.
- DakotaIntVector emptyIntVector
  an empty int vector returned in get functions when there are no variables corresponding to the request.
- DakotaStringArray emptyStringArray
  an empty label array returned in get functions when there are no variables corresponding to the request.

Friends

- int operator== (const FundamentalVariables &vars1, const FundamentalVariables &vars2)
  equality operator.

6.48.1 Detailed Description

Derived class within the DakotaVariables hierarchy which employs the default data view (no variable or 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 FundamentalVariables derived class separates the design, uncertain, and state variable types as well as the continuous and discrete domain types. The result is separate arrays for continuous design, discrete design, uncertain, continuous state, and discrete state variables. This is the default approach, so all iterators and strategies not specifically utilizing the All, Merged, or AllMerged views use this approach (see DakotaVariables::get_variables(problem_db)).

6.48.2 Constructor & Destructor Documentation

6.48.2.1 FundamentalVariables::FundamentalVariables (const ProblemDescDB & *problem_db*)

standard constructor.

Extract fundamental variable types and labels (VariablesUtil is not used).

The documentation for this class was generated from the following files:

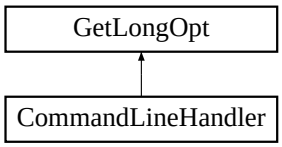
- FundamentalVariables.H
- FundamentalVariables.C

6.49 GetLongOpt Class Reference

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

`#include <CommandLineHandler.H>`

Inheritance diagram for GetLongOpt::



Public Types

- enum OptType { **Valueless**, **OptionalValue**, **MandatoryValue** }
  enum for different types of values associated with command line options.

Public Methods

- 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 (ostream &outfile=cout) const
  Print usage information to outfile.
- void usage (const char *str)
  Change header of usage output to str.

Private Methods

- 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.

6.49.1 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 "=".

6.49.2 Constructor & Destructor Documentation

6.49.2.1 GetLongOpt::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.

6.49.3 Member Function Documentation

6.49.3.1 int GetLongOpt::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.

6.49.3.2 int GetLongOpt::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.

6.49.3.3 int GetLongOpt::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.

6.49.3.4 const char ∗ GetLongOpt::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.

6.49.3.5 void GetLongOpt::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.

The documentation for this class was generated from the following files:

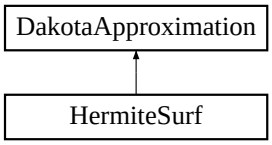
- CommandLineHandler.H
- CommandLineHandler.C

6.50 HermiteSurf Class Reference

Derived approximation class for Hermite polynomials (global approximation).

`#include <HermiteSurf.H>`

Inheritance diagram for HermiteSurf::



Public Methods

- HermiteSurf (const ProblemDescDB &problem_db)

  constructor.

- ~HermiteSurf ()

  destructor.

Protected Methods

- int required_samples (int num_vars)

  return the minimum number of samples required to build the derived class approximation type in num_vars dimensions.

- void find_coefficients ()

  find the Polynomial Chaos coefficients for the response surface.

- Real get_value (const DakotaRealVector &x)

  retrieve the approximate function value for a given parameter vector.

- void get_num_chaos ()

  calculate number of Chaos according to the highest order of Chaos.

Private Methods

- DakotaRealVector get_chaos (const DakotaRealVector &x, int order)

  calculate the Polynomial Chaos from variables.

Private Attributes

- DakotaRealVector chaosCoeffs
  numChaos entries.
- DakotaRealVectorArray chaosSamples
  numChaos∗numCurrentPoints entries.
- int numChaos
  Number of terms in Polynomial Chaos Expansion.
- int highestOrder
  Highest order of Hermite Polynomials in Expansion.

Static Private Attributes

- int index = -1
  index determining which term in the series.

6.50.1 Detailed Description

Derived approximation class for Hermite polynomials (global approximation).

The HermiteSurf class provides a global approximation based on Hermite polynomials. It is used primarily for polynomial chaos expansions (for stochastic finite element approaches to uncertainty quantification).

The documentation for this class was generated from the following files:

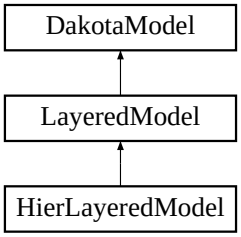
- HermiteSurf.H
- HermiteSurf.C

6.51 HierLayeredModel Class Reference

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

`#include <HierLayeredModel.H>`

Inheritance diagram for HierLayeredModel::



Public Methods

- HierLayeredModel (ProblemDescDB &problem_db)
  constructor.
- ~HierLayeredModel ()
  destructor.

Protected Methods

- void derived_compute_response (const DakotaIntArray &asv)
  portion of compute_response() specific to HierLayeredModel.
- void derived_asynch_compute_response (const DakotaIntArray &asv)
  portion of asynch_compute_response() specific to HierLayeredModel.
- const DakotaArray< DakotaResponse > & derived_synchronize ()
  portion of synchronize() specific to HierLayeredModel.
- const DakotaList< DakotaResponse > & derived_synchronize_nowait ()
  portion of synchronize_nowait() specific to HierLayeredModel.
- DakotaModel & subordinate_model ()
  return highFidelityModel to SurrBasedOptStrategy.
- void build_approximation ()
  use highFidelityModel to compute the truth values needed for correction of lowFidelityInterface results.
- DakotaString local_eval_synchronization ()

return lowFidelityInterface local evaluation synchronization setting.

- const DakotaIntList & synchronize_nowait_completions ()

  return completion id's matching response list from synchronize_nowait (request forwarded to lowFidelityInterface).

- short derived_master_overload () const

  flag which prevents overloading the master with a multiprocessor evaluation (request forwarded to lowFidelityInterface).

- void derived_init_communicators (const DakotaIntArray &message_lengths, const int &max_iterator_concurrency)

  portion of init_communicators() specific to HierLayeredModel (request forwarded to lowFidelityInterface).

- void free_communicators ()

  deallocate communicator partitions for the HierLayeredModel (request forwarded to lowFidelityInterface).

- void serve ()

  Service job requests received from the master. Completes when a termination message is received from stop_servers() (request forwarded to lowFidelityInterface).

- void stop_servers ()

  executed by the master to terminate all slave server operations on a particular model when iteration on that model is complete (request forwarded to lowFidelityInterface).

- int total_eval_counter () const

  return the total evaluation count for the HierLayeredModel (request forwarded to lowFidelityInterface).

- int new_eval_counter () const

  return the new evaluation count for the HierLayeredModel (request forwarded to lowFidelityInterface).

Private Attributes

- DakotaInterface lowFidelityInterface

  manages the approximate low fidelity function evaluations.

- DakotaModel highFidelityModel

  provides truth evaluations for computing corrections to the low fidelity results.

- DakotaResponse highFidResponse

  the high fidelity response is computed in build_approximation() and needs class scope for use in automatic surrogate construction in derived compute_response functions.

- DakotaIntList evalIdList

  bookkeeps fnEvalId's for correction of asynchronous low fidelity evaluations.

6.51.1 Detailed Description

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

The HierLayeredModel class manages hierarchical models of varying fidelity. In particular, it uses a low fidelity model as a surrogate for a high fidelity model. The class contains a lowFidelityInterface which manages the approximate low fidelity function evaluations and a highFidelityModel which provides truth evaluations for computing corrections to the low fidelity results.

6.51.2 Member Function Documentation

6.51.2.1 void HierLayeredModel::derived_compute_response (const DakotaIntArray & *asv*) [protected, virtual]

portion of compute_response() specific to HierLayeredModel.

Evaluate the approximate response using lowFidelityInterface, compute the high fidelity response with build_approximation() (if not performed previously), and, if correction is active, correct the low fidelity results.

Reimplemented from DakotaModel.

6.51.2.2 void HierLayeredModel::derived_asynch_compute_response (const DakotaIntArray & *asv*) [protected, virtual]

portion of asynch_compute_response() specific to HierLayeredModel.

Evaluate the approximate response using an asynchronous lowFidelityInterface mapping and 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 DakotaModel.

6.51.2.3 const DakotaArray< DakotaResponse > & HierLayeredModel::derived_synchronize () [protected, virtual]

portion of synchronize() specific to HierLayeredModel.

Perform a blocking retrieval of all asynchronous evaluations from lowFidelityInterface and, if automatic correction is on, apply correction to each response in the array.

Reimplemented from DakotaModel.

6.51.2.4 const DakotaList< DakotaResponse > & HierLayeredModel::derived_synchronize_nowait () [protected, virtual]

portion of synchronize_nowait() specific to HierLayeredModel.

Perform a nonblocking retrieval of currently available asynchronous evaluations from lowFidelityInterface and, if automatic correction is on, apply correction to each response in the list.

Reimplemented from DakotaModel.

The documentation for this class was generated from the following files:

- HierLayeredModel.H
- HierLayeredModel.C

6.52 KrigApprox Class Reference

Utility class for kriging interpolation.

`#include <KSMSurf.H>`

Public Methods

- KrigApprox (int, int, const DakotaRealVector &, const DakotaRealVector &, const DakotaRealVector &)

  constructor.

- ~KrigApprox ()

  destructor.

- void ModelBuild (int, int, const DakotaRealVector &, const DakotaRealVector &, int)

  Function to compute vector and matrix terms in the kriging surface.

- Real ModelApply (int, int, const DakotaRealVector &)

  Function returns a response value using the kriging surface.

Private Attributes

- 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 conminSingleArray

  Array size parameter needed in interface to CONMIN.

- int numcon

  CONMIN variable: Number of constraints.

- int NFDG

CONMIN variable: Finite difference flag.

- int IPRINT

  CONMIN variable: Flag to control amount of output data.

- int ITMAX

  CONMIN variable: Flag to specify the maximum number of iterations.

- Real FDCH

  CONMIN variable: Relative finite difference step size.

- Real FDCHM

  CONMIN variable: Absolute finite difference step size.

- Real CT

  CONMIN variable: Constraint thickness parameter.

- Real CTMIN

  CONMIN variable: Minimum absolute value of CT used during optimization.

- Real CTL

  CONMIN variable: Constraint thickness parameter for linear and side constraints.

- Real CTLMIN

  CONMIN variable: Minimum value of CTL used during optimization.

- Real DELFUN

  CONMIN variable: Relative convergence criterion threshold.

- Real DABFUN

  CONMIN variable: Absolute convergence criterion threshold.

- int conminInfo

  CONMIN variable: status flag for optimization.

- Real * S

  Internal CONMIN array.

- Real * G1

  Internal CONMIN array.

- Real * G2

  Internal CONMIN array.

- Real * B

  Internal CONMIN array.

- Real * C

  Internal CONMIN array.

- int * MS1

  Internal CONMIN array.

- Real * SCAL

  Internal CONMIN array.

- Real * DF

  Internal CONMIN array.

- Real * A

  Internal CONMIN array.

- int * ISC

  Internal CONMIN array.

- int * IC

  Internal CONMIN array.

- Real * conmin_theta_vars

  Temporary array of design variables used by CONMIN (length N1 = numdv+2).

- Real * conmin_theta_lower_bnds

  Temporary array of lower bounds used by CONMIN (length N1 = numdv+2).

- Real * conmin_theta_upper_bnds

  Temporary array of upper bounds used by CONMIN (length N1 = numdv+2).

- Real ALPHAX

  Internal CONMIN variable: 1-D search parameter.

- Real ABOBJ1

  Internal CONMIN variable: 1-D search parameter.

- Real THETA

  Internal CONMIN variable: mean value of push-off factor.

- Real PHI

  Internal CONMIN variable: "participation coefficient".

- int NSIDE

  Internal CONMIN variable: side constraints parameter.

- int NSCAL

  Internal CONMIN variable: scaling control parameter.

- int NACMX1

  Internal CONMIN variable: estimate of 1+(max # of active constraints).

- int LINOBJ

  Internal CONMIN variable: linear objective function identifier (unused).

- int ITRM

  Internal CONMIN variable: diminishing return criterion iteration number.

- int ICNDIR

  Internal CONMIN variable: conjugate direction restart parameter.

- int IGOTO

  Internal CONMIN variable: internal optimization termination flag.

- int NAC

  Internal CONMIN variable: number of active and violated constraints.

- int INFOG

  Internal CONMIN variable: gradient information flag.

- int ITER

  Internal CONMIN variable: iteration count.

- int iFlag

  Fortran77 flag for kriging computations.

- Real betaHat

  Estimate of the beta term in the kriging model..

- Real maxLikelihoodEst

  Error term computed via Maximum Likelihood Estimation.

- int numNewPts

  Size variable for the arrays used in kriging computations.

- int numSampQuad

  Size variable for the arrays used in kriging computations.

- Real * thetaVector

  Array of correlation parameters for the kriging model.

- Real * xMatrix

  A 2-D array of design points used to build the kriging model.

- Real * yValueVector

  Array of response values corresponding to the array of design points.

- Real * xNewVector

  A 2-D array of design points where the kriging model will be evaluated.

- Real * yNewVector

  Array of response values corresponding to the design points specified in xNewVector.

- Real * thetaLoBndVector

Array of lower bounds in optimizer-to-kriging interface.

- Real * thetaUpBndVector
  Array of upper bounds in optimizer-to-kriging interface.
- Real * constraintVector
  Array of constraint values (used with optimizer).
- Real * rhsTermsVector
  Internal array for kriging Fortran77 code: matrix algebra result.
- int * iPivotVector
  Internal array for kriging Fortran77 code: pivot vector for linear algebra.
- Real * correlationMatrix
  Internal array for kriging Fortran77 code: correlation matrix.
- Real * invcorrelMatrix
  Internal array for kriging Fortran77 code: inverse correlation matrix.
- Real * fValueVector
  Internal array for kriging Fortran77 code: response value vector.
- Real * fRinvVector
  *Internal array for kriging Fortran77 code: vector*matrix result.*
- Real * yfbVector
  Internal array for kriging Fortran77 code: vector arithmetic result.
- Real * yfbRinvVector
  *Internal array for kriging Fortran77 code: vector*matrix result.*
- Real * rXhatVector
  Internal array for kriging Fortran77 code: local correlation vector.
- Real * workVector
  Internal array for kriging Fortran77 code: temporary storage.
- Real * workVectorQuad
  Internal array for kriging Fortran77 code: temporary storage.
- int * iworkVector
  Internal array for kriging Fortran77 code: temporary storage.

6.52.1 Detailed Description

Utility class for kriging interpolation.

The KrigApprox class provides utilities for the KrigingSurf class. It is based on the Ph.D. thesis work of Tony Giunta.

6.52.2 Member Function Documentation

6.52.2.1 Real KrigApprox::ModelApply (int *numVars*, int *numCurrentPoints*, const DakotaRealVector & *x_array*)

Function returns a response value using the kriging surface.

The response value is computed at the design point specified by the DakotaRealVector function argument.

6.52.3 Member Data Documentation

6.52.3.1 int KrigApprox::N1 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N1 = number of variables + 2

6.52.3.2 int KrigApprox::N2 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N2 = number of constraints + 2∗(number of variables)

6.52.3.3 int KrigApprox::N3 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N3 = Maximum possible number of active constraints.

6.52.3.4 int KrigApprox::N4 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N4 = Maximum(N3,number of variables)

6.52.3.5 int KrigApprox::N5 [private]

Size variable for CONMIN arrays. See CONMIN manual.

N5 = 2∗(N4)

6.52.3.6 Real KrigApprox::CT [private]

CONMIN variable: Constraint thickness parameter.

The value of CT decreases in magnitude during optimization.

6.52.3.7 Real* KrigApprox::S [private]

Internal CONMIN array.

Move direction in N-dimensional space.

6.52.3.8 Real* KrigApprox::G1 [private]

Internal CONMIN array.

Temporary storage of constraint values.

6.52.3.9 Real* KrigApprox::G2 [private]

Internal CONMIN array.

Temporary storage of constraint values.

6.52.3.10 Real* KrigApprox::B [private]

Internal CONMIN array.

Temporary storage for computations involving array S.

6.52.3.11 Real* KrigApprox::C [private]

Internal CONMIN array.

Temporary storage for use with arrays B and S.

6.52.3.12 int* KrigApprox::MS1 [private]

Internal CONMIN array.

Temporary storage for use with arrays B and S.

6.52.3.13 Real* KrigApprox::SCAL [private]

Internal CONMIN array.

Vector of scaling parameters for design parameter values.

6.52.3.14 Real* KrigApprox::DF [private]

Internal CONMIN array.

Temporary storage for analytic gradient data.

6.52.3.15 Real* KrigApprox::A [private]

Internal CONMIN array.

Temporary 2-D array for storage of constraint gradients.

6.52.3.16 int* KrigApprox::ISC [private]

Internal CONMIN array.

Array of flags to identify linear constraints. (not used in this implementation of CONMIN)

6.52.3.17 int* KrigApprox::IC [private]

Internal CONMIN array.

Array of flags to identify active and violated constraints

6.52.3.18 int KrigApprox::iFlag [private]

Fortran77 flag for kriging computations.

iFlag=1 computes vector and matrix terms for the kriging surface, iFlag=2 computes the response value (using kriging) at the user-supplied design point.

The documentation for this class was generated from the following files:

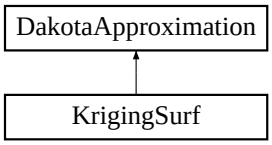
- KSMSurf.H
- KSMSurf.C

6.53 KrigingSurf Class Reference

Derived approximation class for kriging interpolation.

`#include <KSMSurf.H>`

Inheritance diagram for KrigingSurf::



Public Methods

- KrigingSurf (const ProblemDescDB &problem_db)

  constructor.

- ~KrigingSurf ()

  destructor.

Protected Methods

- void find_coefficients ()

  calculate the data fit coefficients using the currentPoints list of SurrogateDataPoints.

- int required_samples (int num_vars)

  return the minimum number of samples required to build the derived class approximation type in num_vars dimensions.

- Real get_value (const DakotaRealVector &x)

  retrieve the approximate function value for a given parameter vector.

Private Attributes

- KrigApprox * krigObject

  Kriging Surface object declaration.

- DakotaRealVector x_matrix

  A 2-d array of all sample sites (design points) used to create the kriging surface.

- DakotaRealVector f_of_x_array

  An array of response values; one response value per sample site.

- DakotaRealVector correlationVector

  An array of correlation parameter values used to build the kriging surface.

- int runConminFlag

  Flag to run CONMIN (value=1) or use user-supplied correlations (value=0).

6.53.1 Detailed Description

Derived approximation class for kriging interpolation.

The KrigingSurf class uses a the kriging approach to interpolate between data points. It is based on the Ph.D. thesis work of Tony Giunta.

The documentation for this class was generated from the following files:

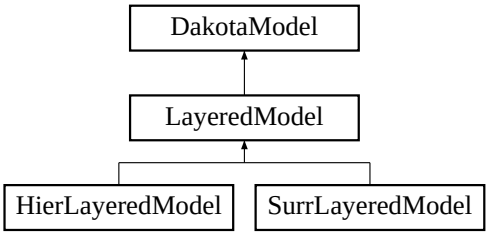
- KSMSurf.H
- KSMSurf.C

6.54 LayeredModel Class Reference

Base class for the layered models (SurrLayeredModel and HierLayeredModel).

`#include <LayeredModel.H>`

Inheritance diagram for LayeredModel::



Protected Methods

- LayeredModel (ProblemDescDB &problem_db)

  constructor.

- ~LayeredModel ()

  destructor.

- void compute_correction (const DakotaResponse &truth_response, const DakotaResponse &approx_response, const DakotaRealVector &c_vars)

  compute the correction required to bring approx_response into agreement with truth_response.

- void apply_correction (DakotaResponse &approx_response, const DakotaRealVector &c_vars, short quiet_flag=0)

  apply the correction computed in compute_correction() to approx_response.

- void check_submodel_compatibility (const DakotaModel &sub_model)

  verify compatibility between LayeredModel attributes and attributes of the submodel (SurrLayeredModel::actualModel or HierLayeredModel::highFidelityModel).

- void auto_correction (short correction_flag)

  sets autoCorrection to ON (1) or OFF (0).

Protected Attributes

- DakotaArray< DakotaResponse > correctedResponseArray

  array of corrected responses used in derived_synchronize() functions.

- DakotaList< DakotaResponse > correctedResponseList

  list of corrected responses used in derived_synchronize_nowait() functions.

- DakotaList< DakotaRealVector > rawCVarsList

  list of raw continuous variables used by apply_correction(). DakotaModel::varsList cannot be used for this purpose since it does not contain lower level variables sets from finite differencing.

- DakotaString correctionType

  correction approach to be used: offset, scaled, or beta.

- int approxBuilds

  number of calls to build_approximation().

- short autoCorrection

  a flag which controls the use of apply_correction() in SurrLayeredModel and HierLayeredModel approximate response computations.

Private Attributes

- DakotaRealVector offsetValues

  values with which to offset the function values in an approximate response in order to apply a truth model correction.

- DakotaRealVector scaleFactors

  values with which to scale the function values, gradients, and Hessians in an approximate response in order to apply a truth model correction.

- short correctionComputed

  flag used to indicate whether or not a correction is available.

- short badScalingFlag

  flag used to indicate function values near zero for scaled corrections; triggers an automatic switch from scaled to offset correction.

- DakotaRealVector betaFcnRatio

  Beta-correction scaling term: ratio of high-fidelity model value to low fidelity value at x=x_center.

- DakotaRealMatrix betaGrads

  Beta-correction scaling term: gradient of beta at x=x_center.

- DakotaRealVector betaCenterPt

  Beta-correction scaling term: center point of the trust region.

- DakotaRealVector betaApproxCenterVals

  Function values at the center of the trust region which are needed as a fall back if the current function values are unavailable when applying the beta-correction.

- DakotaRealMatrix betaApproxCenterGrads

  Gradient values at the center of the trust region which are needed as a fall back if the current function gradients are unavailable when applying the beta-correction.

- DakotaRealMatrix betaGradOffset

  Beta-correction scaling term: gradient offsets.

- DakotaRealVector betaHessOffset

  Beta-correction scaling term: Hessian offsets.

6.54.1 Detailed Description

Base class for the layered models (SurrLayeredModel and HierLayeredModel).

The LayeredModel class provides common functions to derived classes for computing and applying corrections to approximations.

6.54.2 Member Function Documentation

6.54.2.1 void LayeredModel::compute_correction (const DakotaResponse & *truth_response*, const DakotaResponse & *approx_response*, const DakotaRealVector & *c_vars*) [protected, virtual]

compute the correction required to bring approx_response into agreement with truth_response.

Compute a correction for approximate responses based on an offset, scaled, or beta correction approach. The offset and scaled approaches will correct the approximate function values to match the truth function values at a single point in the parameter space (e.g., the center of a trust region). In the "beta" correction approach, the function value and the function gradient are matched at a single point. The beta-correction is similar to the scaled-correction method, but the scaled-correction uses a scalar value for each response function, whereas the beta-correction uses a ***scaling function*** for each response function that varies w.r.t. position in the parameter space.

Reimplemented from DakotaModel.

6.54.3 Member Data Documentation

6.54.3.1 int LayeredModel::approxBuilds [protected]

number of calls to build_approximation().

used as a flag to automatically build the approximation if one of the derived compute_response functions is called prior to build_approximation().

6.54.3.2 short LayeredModel::autoCorrection [protected]

a flag which controls the use of apply_correction() in SurrLayeredModel and HierLayeredModel approximate response computations.

the default is ON once compute_correction() has been called. However this should be overridden when a new correction is desired, since compute_correction() no longer automatically backs out an old correction.

The documentation for this class was generated from the following files:

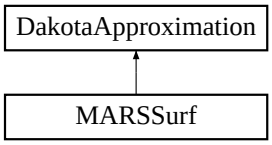
- LayeredModel.H
- LayeredModel.C

6.55 MARSSurf Class Reference

Derived approximation class for multivariate adaptive regression splines.

`#include <MARSSurf.H>`

Inheritance diagram for MARSSurf::



Public Methods

- MARSSurf (const ProblemDescDB &problem_db)

  constructor.

- ~MARSSurf ()

  destructor.

Protected Methods

- int required_samples (int num_vars)

  return the minimum number of samples required to build the derived class approximation type in num_vars dimensions.

- void find_coefficients ()

  calculate the data fit coefficients using the currentPoints list of SurrogateDataPoints.

- Real get_value (const DakotaRealVector &x)

  retrieve the approximate function value for a given parameter vector.

Private Attributes

- int * flags

  variable type declarations (ordinal, excluded, categorical).

- Mars * marsObject

  pointer to the Mars object (MARS wrapper provided as part of DDACE).

6.55.1 Detailed Description

Derived approximation class for multivariate adaptive regression splines.

The MARSSurf class provides a global approximation based on regression splines. It employs the C++ wrapper developed by the DDACE team for the Multivariate Adaptive Regression Splines (MARS) package from Prof. Jerome Friedman of Stanford University Dept. of Statistics.

The documentation for this class was generated from the following files:

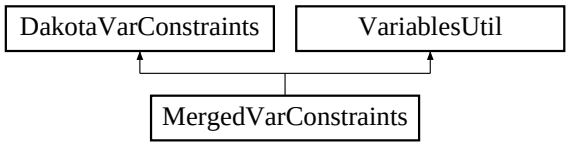
- MARSSurf.H
- MARSSurf.C

6.56 MergedVarConstraints Class Reference

Derived class within the DakotaVarConstraints hierarchy which employs the merged data view.

`#include <MergedVarConstraints.H>`

Inheritance diagram for MergedVarConstraints::



Public Methods

- MergedVarConstraints (const ProblemDescDB &problem_db)
  constructor.
- ~MergedVarConstraints ()
  destructor.
- const DakotaRealVector & continuous_lower_bounds () const
  return the active continuous variable lower bounds.
- void continuous_lower_bounds (const DakotaRealVector &c_l_bnds)
  set the active continuous variable lower bounds.
- const DakotaRealVector & continuous_upper_bounds () const
  return the active continuous variable upper bounds.
- void continuous_upper_bounds (const DakotaRealVector &c_u_bnds)
  set the active continuous variable upper bounds.
- const DakotaIntVector & discrete_lower_bounds () const
  return the active discrete variable lower bounds.
- void discrete_lower_bounds (const DakotaIntVector &d_l_bnds)
  set the active discrete variable lower bounds.
- const DakotaIntVector & discrete_upper_bounds () const
  return the active discrete variable upper bounds.
- void discrete_upper_bounds (const DakotaIntVector &d_u_bnds)
  set the active discrete variable upper bounds.
- void write (ostream &s) const

write a variable constraints object to an ostream.

- void read (istream &s)

  read a variable constraints object from an istream.

Private Attributes

- DakotaRealVector mergedDesignLowerBnds

  a design lower bounds array merging continuous and discrete domains (integer values promoted to reals).

- DakotaRealVector mergedDesignUpperBnds

  a design upper bounds array merging continuous and discrete domains (integer values promoted to reals).

- DakotaRealVector uncertainDistLowerBnds

  the uncertain distribution lower bounds array (no discrete uncertain to merge).

- DakotaRealVector uncertainDistUpperBnds

  the uncertain distribution upper bounds array (no discrete uncertain to merge).

- DakotaRealVector mergedStateLowerBnds

  a state lower bounds array merging continuous and discrete domains (integer values promoted to reals).

- DakotaRealVector mergedStateUpperBnds

  a state upper bounds array merging continuous and discrete domains (integer values promoted to reals).

- DakotaIntVector emptyIntVector

  an empty int vector returned in get functions when there are no variables corresponding to the request.

6.56.1 Detailed Description

Derived class within the DakotaVarConstraints hierarchy which employs the merged data view.

Derived variable constraints classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The MergedVarConstraints derived class combines continuous and discrete domain types but separates design, uncertain, and state variable types. The result is merged design bounds arrays (mergedDesignLowerBnds, mergedDesignUpperBnds), uncertain distribution bounds arrays (uncertainDistLowerBnds, uncertainDistUpperBnds), and merged state bounds arrays (mergedStateLowerBnds, mergedStateUpperBnds). The branch and bound strategy uses this approach (see DakotaVariables::get_variables(problem_db) for variables type selection; variables type is passed to the DakotaVarConstraints constructor in DakotaModel).

6.56.2 Constructor & Destructor Documentation

6.56.2.1 MergedVarConstraints::MergedVarConstraints (const ProblemDescDB & *problem_db*)

constructor.

Extract fundamental lower and upper bounds and merge continuous and discrete domains to create mergedDesignLowerBnds, mergedDesignUpperBnds, mergedStateLowerBnds, and mergedStateUpperBnds using utilities from VariablesUtil (uncertain distribution bounds do not require any merging).

The documentation for this class was generated from the following files:

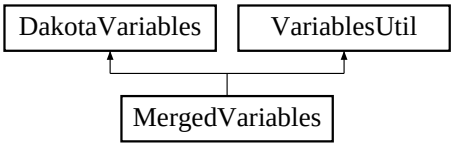
- MergedVarConstraints.H
- MergedVarConstraints.C

6.57 MergedVariables Class Reference

Derived class within the DakotaVariables hierarchy which employs the merged data view.

`#include <MergedVariables.H>`

Inheritance diagram for MergedVariables::



Public Methods

- MergedVariables ()
  default constructor.
- MergedVariables (const ProblemDescDB &problem_db)
  standard constructor.
- ~MergedVariables ()
  destructor.
- size_t tv () const
  Returns total number of vars.
- size_t cv () const
  Returns number of active continuous vars.
- size_t dv () const
  Returns number of active discrete vars.
- const DakotaRealVector & continuous_variables () const
  return the active continuous variables.
- void continuous_variables (const DakotaRealVector &c_vars)
  set the active continuous variables.
- const DakotaIntVector & discrete_variables () const
  return the active discrete variables.
- void discrete_variables (const DakotaIntVector &d_vars)
  set the active discrete variables.
- const DakotaStringArray & continuous_variable_labels () const

return the active continuous variable labels.

- void continuous_variable_labels (const DakotaStringArray &cv_labels)
  set the active continuous variable labels.
- const DakotaStringArray & discrete_variable_labels () const
  return the active discrete variable labels.
- void discrete_variable_labels (const DakotaStringArray &dv_labels)
  set the active discrete variable labels.
- const DakotaRealVector & inactive_continuous_variables () const
  return the inactive continuous variables.
- void inactive_continuous_variables (const DakotaRealVector &i_c_vars)
  set the inactive continuous variables.
- const DakotaIntVector & inactive_discrete_variables () const
  return the inactive discrete variables.
- void inactive_discrete_variables (const DakotaIntVector &i_d_vars)
  set the inactive discrete variables.
- size_t acv () const
  returns total number of continuous vars.
- size_t adv () const
  returns total number of discrete vars.
- DakotaRealVector all_continuous_variables () const
  returns a single array with all continuous variables.
- DakotaIntVector all_discrete_variables () const
  returns a single array with all discrete variables.
- void read (istream &s)
  read a variables object from an istream.
- void write (ostream &s) const
  write a variables object to an ostream.
- void read_annotated (istream &s)
  read a variables object in annotated format from an istream.
- void write_annotated (ostream &s) const
  write a variables object in annotated format to an ostream.
- void read (DakotaBiStream &s)
  read a variables object from the binary restart stream.

- void write (DakotaBoStream &s) const

  write a variables object to the binary restart stream.

- void read (UnPackBuffer &s)

  read a variables object from a packed MPI buffer.

- void write (PackBuffer &s) const

  write a variables object to a packed MPI buffer.

Private Methods

- void copy_rep (const DakotaVariables *vars_rep)

  Used by copy() to copy the contents of a letter class.

Private Attributes

- DakotaRealVector mergedDesignVars

  a design variables array merging continuous and discrete domains (integer values promoted to reals).

- DakotaRealVector uncertainVars

  the uncertain variables array (no discrete uncertain to merge).

- DakotaRealVector mergedStateVars

  a state variables array merging continuous and discrete domains (integer values promoted to reals).

- DakotaStringArray mergedDesignLabels

  a label array combining continuous design and discrete design labels.

- DakotaStringArray uncertainLabels

  the uncertain variables label array (no discrete uncertain to combine).

- DakotaStringArray mergedStateLabels

  a label array combining continuous state and discrete state labels.

- DakotaIntVector emptyIntVector

  an empty int vector returned in get functions when there are no variables corresponding to the request.

- DakotaStringArray emptyStringArray

  an empty label array returned in get functions when there are no variables corresponding to the request.

Friends

- int operator== (const MergedVariables &vars1, const MergedVariables &vars2)

  equality operator.

6.57.1 Detailed Description

Derived class within the DakotaVariables hierarchy which employs the merged data view.

Derived variables classes take different views of the design, uncertain, and state variable types and the continuous and discrete domain types. The MergedVariables derived class combines continuous and discrete domain types but separates design, uncertain, and state variable types. The result is a single continuous array of design variables (mergedDesignVars), a single continuous array of uncertain variables (uncertainVars), and a single continuous array of state variables (mergedStateVars). The branch and bound strategy uses this approach (see DakotaVariables::get_variables(problem_db)).

6.57.2 Constructor & Destructor Documentation

6.57.2.1 MergedVariables::MergedVariables (const ProblemDescDB & *problem_db*)

standard constructor.

Extract fundamental variable types and labels and merge continuous and discrete domains to create mergedDesignVars, mergedStateVars, mergedDesignLabels, and mergedStateLabels using utilities from VariablesUtil (uncertain variables and labels do not require any merging).

The documentation for this class was generated from the following files:

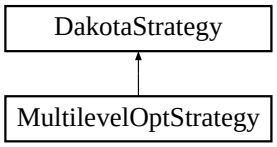
- MergedVariables.H
- MergedVariables.C

6.58 MultilevelOptStrategy Class Reference

Strategy for hybrid optimization using multiple optimizers on multiple models of varying fidelity.

`#include <MultilevelOptStrategy.H>`

Inheritance diagram for MultilevelOptStrategy::



Public Methods

- MultilevelOptStrategy (ProblemDescDB &problem_db)

  constructor.

- ~MultilevelOptStrategy ()

  destructor.

- void run_strategy ()

  Performs the hybrid optimization strategy by executing multiple iterators on different models of varying fidelity.

Private Methods

- void run_coupled ()

  run a tightly coupled hybrid.

- void run_uncoupled ()

  run an uncoupled hybrid.

- void run_uncoupled_adaptive ()

  run an uncoupled adaptive hybrid.

Private Attributes

- DakotaString multiLevelType

  coupled, uncoupled, or uncoupled_adaptive.

- DakotaStringList methodList

  the list of method identifiers.

- int numIterators

  number of methods in methodList.

- Real localSearchProb

  the probability of running a local search refinement within phases of the global optimization for coupled hybrids.

- Real progressMetric

  the amount of progress made in a single iterator++ cycle within an uncoupled adaptive hybrid.

- Real progressThreshold

  when the progress metric falls below this threshold, the uncoupled adaptive hybrid switches to the next method.

- DakotaArray< DakotaIterator > selectedIterators

  the set of iterators, one for each entry in methodList.

- DakotaArray< DakotaModel > userDefinedModels

  the set of models, one for each iterator.

6.58.1 Detailed Description

Strategy for hybrid optimization using multiple optimizers on multiple models of varying fidelity.

This strategy has three approaches to hybrid optimization: (1) the uncoupled 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; (2) the uncoupled adaptive hybrid is similar to the uncoupled hybrid, except that the stopping rules for the optimizers are controlled adapatively by the strategy instead of internally by each optimizer; and (3) the coupled hybrid uses multiple methods in close coordination, generally using a local search optimizer repeatedly within a global optimizer (the local search optimizer refines candidate optima which are fed back to the global optimizer). The uncoupled strategies only pass information forward, whereas the coupled strategy allows both feed forward and feedback. Note that while the strategy is targeted at optimizers, any iterator may be used so long as it defines the notion of a final solution which can be passed as the starting point for subsequent iterators.

6.58.2 Member Function Documentation

6.58.2.1 void MultilevelOptStrategy::run_coupled () [private]

run a tightly coupled hybrid.

In the coupled case, use is made of external hybridization capabilities, such as those available in the global/local hybrids from SGOPT. This function is responsible only for publishing the local optimizer selection to the global optimizer and then invoking the global optimizer; the logic of method switching is handled entirely within the global optimizer. Status: incomplete.

6.58.2.2 void MultilevelOptStrategy::run_uncoupled () [private]

run an uncoupled hybrid.

In the uncoupled nonadaptive case, there is no interference with the iterators. Each runs until its own convergence criteria is satisfied (using iterator.run_iterator()). Status: fully operational.

6.58.2.3 void MultilevelOptStrategy::run_uncoupled_adaptive () [private]

run an uncoupled adaptive hybrid.

In the uncoupled 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.

The documentation for this class was generated from the following files:

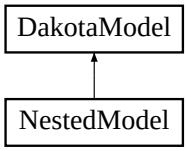
- MultilevelOptStrategy.H
- MultilevelOptStrategy.C

6.59 NestedModel Class Reference

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

`#include <NestedModel.H>`

Inheritance diagram for NestedModel::



Public Methods

- NestedModel (ProblemDescDB &problem_db)
  constructor.
- ~NestedModel ()
  destructor.

Protected Methods

- void derived_compute_response (const DakotaIntArray &asv)
  portion of compute_response() specific to NestedModel.
- void derived_asynch_compute_response (const DakotaIntArray &asv)
  portion of asynch_compute_response() specific to NestedModel.
- const DakotaArray< DakotaResponse > & derived_synchronize ()
  portion of synchronize() specific to NestedModel.
- const DakotaList< DakotaResponse > & derived_synchronize_nowait ()
  portion of synchronize_nowait() specific to NestedModel.
- const DakotaIntList & synchronize_nowait_completions ()
  Return completion id's matching response list from synchronize_nowait.
- DakotaModel & subordinate_model ()
  return a reference to the subModel.
- short derived_master_overload () const
  flag which prevents overloading the master with a multiprocessor evaluation (forwarded to subModel so that UQ portion of OUU can execute in parallel).

- void derived_init_communicators (const DakotaIntArray &message_lengths, const int &max_iterator_concurrency)

  portion of init_communicators() specific to NestedModel.

- void free_communicators ()

  deallocate communicator partitions for the NestedModel (forwarded to subModel so that UQ portion of OUU can execute in parallel).

- void serve ()

  Service job requests received from the master. Completes when a termination message is received from stop_servers(). (forwarded to subModel so that UQ portion of OUU can execute in parallel).

- void stop_servers ()

  Executed by the master to terminate all slave server operations on a particular model when iteration on that model is complete (forwarded to subModel so that UQ portion of OUU can execute in parallel).

- int total_eval_counter () const

  Return the total evaluation count for the NestedModel; forwarded to optionalInterface if present (placeholder for now).

- int new_eval_counter () const

  Return the new evaluation count for the NestedModel; forwarded to optionalInterface if present (placeholder for now).

Private Methods

- void response_mapping (const DakotaResponse &interface_response, const DakotaResponse &sub_iterator_response, DakotaResponse &mapped_response)

  combine the response from the optional interface evaluation with the response from the sub-iteration using the objCoeffs/constrCoeffs mappings to create the total response for the model.

- void asv_mapping (const DakotaIntArray &mapped_asv, DakotaIntArray &interface_asv)

  define the evaluation requirements for the optional interface (interface_asv) from the total model evaluation requirements (mapped_asv).

Private Attributes

- DakotaIterator subIterator

  the sub-iterator that is executed on every evaluation of this model.

- DakotaModel subModel

  the sub-model used in sub-iterator evaluations.

- size_t numSubIteratorIneqConstr

  number of top-level inequality constraints mapped from the sub-iteration results.

- size_t numSubIteratorEqConstr

number of top-level equality constraints mapped from the sub-iteration results.

- DakotaInterface optionalInterface

  the optional interface contributes nonnested response data to the total model response.

- DakotaString interfacePointer

  the optional interface pointer from the nested model specification.

- DakotaResponse interfaceResponse

  the response object resulting from optional interface evaluations.

- size_t numInterfObjFns

  number of objective functions resulting from optional interface evaluations.

- size_t numInterfIneqConstr

  number of inequality constraints resulting from optional interface evaluations.

- size_t numInterfEqConstr

  number of equality constraints resulting from the optional interface evaluations.

- DakotaRealMatrix objCoeffs

  "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 function(s).

- DakotaRealMatrix constrCoeffs

  "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.

- DakotaArray< DakotaResponse > responseArray

  dummy response array for derived_synchronize() prior to derived_asynch_compute_response() support.

- DakotaList< DakotaResponse > responseList

  dummy response list for derived_synchronize_nowait() prior to derived_asynch_compute_response() support.

- DakotaIntList completionList

  dummy completion list for synchronize_nowait_completions() prior to derived_asynch_compute_response() support.

6.59.1 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.

6.59.2 Member Function Documentation

6.59.2.1 void NestedModel::derived_compute_response (const DakotaIntArray & *asv*) [protected, virtual]

portion of compute_response() 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 DakotaModel.

6.59.2.2 void NestedModel::derived_asynch_compute_response (const DakotaIntArray & *asv*) [protected, virtual]

portion of asynch_compute_response() specific to NestedModel.

Not currently supported by NestedModels (need to add concurrent iterator support). As a result, derived_synchronize(), derived_synchronize_nowait(), and synchronize_nowait_completions() are inactive as well).

Reimplemented from DakotaModel.

6.59.2.3 const DakotaArray< DakotaResponse > & NestedModel::derived_synchronize () [protected, virtual]

portion of synchronize() specific to NestedModel.

Asynchronous response computations are not currently supported by NestedModels. Return a dummy responseArray to satisfy the compiler.

Reimplemented from DakotaModel.

6.59.2.4 const DakotaList< DakotaResponse > & NestedModel::derived_synchronize_nowait () [protected, virtual]

portion of synchronize_nowait() specific to NestedModel.

Asynchronous response computations are not currently supported by NestedModels. Return a dummy responseList to satisfy the compiler.

Reimplemented from DakotaModel.

6.59.2.5 const DakotaIntList & NestedModel::synchronize_nowait_completions () [inline, protected, virtual]

Return completion id's matching response list from synchronize_nowait.

Asynchronous response computations are not currently supported by NestedModels. Return a dummy completionList to satisfy the compiler.

Reimplemented from DakotaModel.

6.59.2.6 void NestedModel::derived_init_communicators (const DakotaIntArray & *message_lengths*, const int & *max_iterator_concurrency*) [inline, protected, virtual]

portion of init_communicators() specific to NestedModel.

Asynchronous flags need to be initialized for the subModel. In addition, max_iterator_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 DakotaModel.

6.59.2.7 void NestedModel::response_mapping (const DakotaResponse & *interface_response*, const DakotaResponse & *sub_iterator_response*, DakotaResponse & *mapped_response*) [private]

combine the response from the optional interface evaluation with the response from the sub-iteration using the objCoeffs/constrCoeffs mappings to create the total response for the model.

In the OUU case,

```
optionalInterface functions = {f}, {g}  (deterministic objectives & constraints)
subIterator functions       = {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 (objCoeffs class attribute), [A] is the secondary_mapping_matrix user input (constrCoeffs 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 objectives overlap but optionalInterface/subIterator constraints do not. The [W] matrix can be specified so as to allow

- some purely deterministic objective 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 objective functions: [W] filled and [W].num_rows() > {f}.length()
- separate deterministic and stochastic objective 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.

6.59.3 Member Data Documentation

6.59.3.1 DakotaModel NestedModel::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 LayeredModels and vice versa.

The documentation for this class was generated from the following files:

- NestedModel.H
- NestedModel.C

6.60 NoDBBaseConstructor Struct Reference

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

`#include <ProblemDescDB.H>`

Public Methods

- NoDBBaseConstructor (int=0)

  C++ structs can have constructors.

6.60.1 Detailed Description

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

NoDBBaseConstructor is used to overload the constructor used for on-the-fly iterator instantiations in which ProblemDescDB queries cannot be used. Putting this struct here (rather than in a header of a class that uses it) avoids problems with circular dependencies.

The documentation for this struct was generated from the following file:

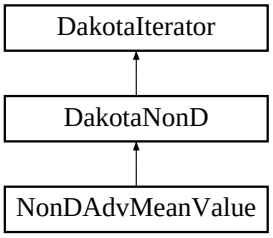
- ProblemDescDB.H

6.61 NonDAdvMeanValue Class Reference

Class for the analytical reliability methods within DAKOTA/UQ.

`#include <NonDAdvMeanValue.H>`

Inheritance diagram for NonDAdvMeanValue::



Public Methods

- NonDAdvMeanValue (DakotaModel &model)

  constructor.

- ~NonDAdvMeanValue ()

  destructor.

- void quantify_uncertainty ()

  performs an uncertainty propagation using analytical reliability methods which solve constrained optimization problems to obtain approximations of the cumulative distribution function of response.

- void print_iterator_results (ostream &s) const

  print the approximate mean,standard deviation, and importance factors when using the mean value method (MV) or the CDF information when using other reliability methods (AMV,AMV+,FORM).

Static Private Methods

- void lin_approx_objective_eval (int &mode, int &n, Real *u, Real &f, Real *gradf, int &)

  static function used by NPSOL as the objective function in the constrained optimization problems solved in the analytical reliability methods.

- void lin_approx_constraint_eval (int &mode, int &ncnln, int &n, int &nrowj, int *needc, Real *u, Real *c, Real *cjac, int &nstate)

  static function used by NPSOL as the constraint function in the constrained optimization problems solved in the analytical reliability methods.

- void transUToX (const Epetra_SerialDenseVector &uncorr_normal_vars, Epetra_SerialDenseVector &random_vars)

  Transformation Routine from u-space of random variables to x-space of random variables for Petra data types.

- void transUToX (const DakotaRealVector &uncorr_normal_vars, DakotaRealVector &random_vars)

  Transformation Routine from u-space of random variables to x-space of random variables for DakotaRealVector data types.

- void transXToU (const Epetra_SerialDenseVector &random_vars, Epetra_SerialDenseVector &uncorr_normal_vars)

  Transformation Routine from x-space of random variables to u-space of random variables for Petra data types.

- void transXToZ (const Epetra_SerialDenseVector &random_vars, Epetra_SerialDenseVector &correlated_normal_vars)

  Transformation Routine from x-space of random variables to z-space of random variables for Petra data types.

- void transUToZ (const Epetra_SerialDenseVector &uncorr_normal_vars, Epetra_SerialDenseVector &correlated_normal_vars)

  Transformation Routine from u-space of random variables to z-space of random variables for Petra data types.

- void transZToU (Epetra_SerialDenseVector &correlated_normal_vars, Epetra_SerialDenseVector &uncorr_normal_vars)

  Transformation Routine from z-space of random variables to u-space of random variables for Petra data types.

- void jacXToZ (const Epetra_SerialDenseVector &random_vars, const Epetra_SerialDenseVector &correlated_normal_vars, Epetra_SerialDenseMatrix &jacobianXZ)

  Jacobian of mapping from x to z random variable space.

- void jacZToX (const Epetra_SerialDenseVector &correlated_normal_vars, const Epetra_SerialDenseVector &random_vars, Epetra_SerialDenseMatrix &jacobianZX)

  Jacobian of mapping from z to x random variable space.

- void jacXToU (const Epetra_SerialDenseVector &random_vars, const Epetra_SerialDenseVector &uncorr_normal_vars, Epetra_SerialDenseMatrix &jacobianXU)

  Jacobian of mapping from x to u random variable space.

- void jacUToX (const Epetra_SerialDenseVector &uncorr_normal_vars, const Epetra_SerialDenseVector &random_vars, Epetra_SerialDenseMatrix &jacobianUX)

  Jacobian of mapping from u to x random variable space.

- void transNataf (Epetra_SerialSymDenseMatrix &mod_corr_matrix)

  This procedure modifys the correlation matrix input by the user to be used in the Nataf distribution model.

- void erfInverse (const double &p, double &z)

  Inverse of error function used to invert cdf of normal random variables.

Private Attributes

- DakotaString reliabilityMethod
  reliability method identifier specified by user specifies amvFlag.
- DakotaRealArray responseLevelTargets
  user specified targets for response levels.
- DakotaRealArray probabilityLevelTargets
  user specified targets for probability levels.
- DakotaRealVector meanResponse
  approximate mean values of response functions predicted by MV.
- DakotaRealVector stdResponse
  approximate standard deviations of response functions predicted by MV.
- DakotaRealMatrix impFactor
  importance factors predicted by MV.

Static Private Attributes

- Epetra_SerialDenseVector staticFnVals
  static copy of DakotaResponseRep::functionValues.
- Epetra_SerialDenseMatrix staticFnGrads
  static copy of DakotaResponseRep::functionGradients.
- Epetra_SerialDenseMatrix staticGlobalGradsX
  Gradient of Response function in x-sapce for each response level.
- Epetra_SerialDenseMatrix staticGlobalGradsU
  Gradient of Response function in u-space for each response level.
- Epetra_SerialSymDenseMatrix petraCorrMatrix
  petra copy of uncertainCorrelations.
- Epetra_SerialDenseMatrix cholCorrMatrix
  cholesky factor of petraCorrMatrix.
- Epetra_SerialDenseMatrix mostProbPointX
  Location of MPP in x space.
- Epetra_SerialDenseMatrix mostProbPointU
  Location of MPP in u space.
- Epetra_SerialDenseVector ranVarMeans
  Mean Vector of all uncertain random variables.

- Epetra_SerialDenseVector ranVarSigmas

  Standard Deviation Vector of all uncertain random variables.

- Epetra_SerialDenseVector petraRespLevels

  Petra copy of responseLevelTargets specified by user.

- Epetra_SerialDenseVector petraProbLevels

  Petra copy of probabilityLevelTargets specified by user.

- Epetra_SerialDenseVector correctedRespLevel

  output response levels calculated.

- int respLevelCount

  counter for which response level is being analyzed.

- int amvFlag

  flag to represent which reliability method is being used.

- size_t staticNumUncVars

  static copy of numUncertainVars.

- size_t staticNumFuncs

  static copy of numFunctions.

- DakotaIntVector ranVarType

  vector of indices indicating which type of uncertain variable.

- DakotaRealVector medianFnVals

  vector of median values of functions used to determine which side of probability equal 0.5 the response level is.

- DakotaRealVector probLevels

  computed probability values.

6.61.1 Detailed Description

Class for the analytical reliability methods within DAKOTA/UQ.

The NonDAdvMeanValue class implements the following analytic reliability methods: advanced mean value method (AMV), iterated advanced mean value method (AMV+), first order reliability method (FORM), and second order reliability method (SORM). Each of these employ an optimizer (currently NPSOL) to perform a search for the most probable point (MPP).

6.61.2 Member Function Documentation

6.61.2.1 void NonDAdvMeanValue::lin_approx_objective_eval (int & *mode*, int & *n*, Real * *u*, Real & *f*, Real * *gradf*, int &) [static, private]

static function used by NPSOL as the objective function in the constrained optimization problems solved in the analytical reliability methods.

Need to be static so that they can be passed in function pointers without having to restrict the recipient to functions from the NonDAdvMeanValue class (see Stroustrup, p.166 - pointers to member functions must use class scope operators which would restrict the generality of the NPSOLOptimizer "user_functions" interface).

6.61.2.2 void NonDAdvMeanValue::lin_approx_constraint_eval (int & *mode*, int & *ncnln*, int & *n*, int & *nrowj*, int * *needc*, Real * *u*, Real * *c*, Real * *cjac*, int & *nstate*) [static, private]

static function used by NPSOL as the constraint function in the constrained optimization problems solved in the analytical reliability methods.

Need to be static so that they can be passed in function pointers without having to restrict the recipient to functions from the NonDAdvMeanValue class (see Stroustrup, p.166 - pointers to member functions must use class scope operators which would restrict the generality of the NPSOLOptimizer "user_functions" interface).

6.61.2.3 void NonDAdvMeanValue::transUToX (const Epetra_SerialDenseVector & *uncorr_normal_vars*, Epetra_SerialDenseVector & *random_vars*) [static, private]

Transformation Routine from u-space of random variables to x-space of random variables for Petra data types.

This procedure performs the transformation from u to x space

uncorr_normal_vars is the vector of random variables in standard normal space (u-space).

random_vars is the vector of the random variables in the user-defined x-space

6.61.2.4 void NonDAdvMeanValue::transXToU (const Epetra_SerialDenseVector & *random_vars*, Epetra_SerialDenseVector & *uncorr_normal_vars*) [static, private]

Transformation Routine from x-space of random variables to u-space of random variables for Petra data types.

This procedure performs the transformation from x to u space

uncorr_normal_vars is the vector of random variables in standard normal space (u-space).

random_vars is the vector of the random variables in the user-defined x-space

6.61.2.5 void NonDAdvMeanValue::transXToZ (const Epetra_SerialDenseVector & *random_vars*, Epetra_SerialDenseVector & *correlated_normal_vars*) [static, private]

Transformation Routine from x-space of random variables to z-space of random variables for Petra data types.

This procedure performs the transformation from x to z space

correlated_normal_vars is the vector of random variables in normal space with proper correlations(z-space).

random_vars is the vector of the random variables in the user-defined x-space

6.61.2.6 void NonDAdvMeanValue::transUToZ (const Epetra_SerialDenseVector & *uncorr_normal_vars*, Epetra_SerialDenseVector & *correlated_normal_vars*) [static, private]

Transformation Routine from u-space of random variables to z-space of random variables for Petra data types.

This procedure computes the transformation from u to z space.

uncorr_normal_vars is the vector of random variables in standard normal space (u-space).

correlated_normal_vars is the vector of random variables in normal space with proper correlations(z-space).

6.61.2.7 void NonDAdvMeanValue::transZToU (Epetra_SerialDenseVector & *correlated_normal_vars*, Epetra_SerialDenseVector & *uncorr_normal_vars*) [static, private]

Transformation Routine from z-space of random variables to u-space of random variables for Petra data types.

This procedure computes the transformation from z to u space.

uncorr_normal_vars is the vector of random variables in standard normal space (u-space).

correlated_normal_vars is the vector of random variables in normal space with proper correlations(z-space).

6.61.2.8 void NonDAdvMeanValue::jacXToZ (const Epetra_SerialDenseVector & *random_vars*, const Epetra_SerialDenseVector & *correlated_normal_vars*, Epetra_SerialDenseMatrix & *jacobianXZ*) [static, private]

Jacobian of mapping from x to z random variable space.

This procedure computes the jacobian of the transformation from x to z space.

correlated_normal_vars is the vector of random variables in normal space with proper correlations (z-space).

random_vars is the vector of the random variables in the user-defined x-space.

6.61.2.9 void NonDAdvMeanValue::jacZToX (const Epetra_SerialDenseVector & *correlated_normal_vars*, const Epetra_SerialDenseVector & *random_vars*, Epetra_SerialDenseMatrix & *jacobianZX*) [static, private]

Jacobian of mapping from z to x random variable space.

This procedure computes the jacobian of the transformation from z to x space.

correlated_normal_vars is the vector of random variables in normal space with proper correlations (z-space).

random_vars is the vector of the random variables in the user-defined x-space.

6.61.2.10 void NonDAdvMeanValue::jacXToU (const Epetra_SerialDenseVector & *random_vars*, const Epetra_SerialDenseVector & *uncorr_normal_vars*, Epetra_SerialDenseMatrix & *jacobianXU*) [static, private]

Jacobian of mapping from x to u random variable space.

This procedure computes the jacobian of the transformation from x to u space.

uncorr_normal_vars is the vector of random variables in standard normal space (u-space).

random_vars is the vector of the random variables in the user-defined x-space

6.61.2.11 void NonDAdvMeanValue::jacUToX (const Epetra_SerialDenseVector & *uncorr_normal_vars*, const Epetra_SerialDenseVector & *random_vars*, Epetra_SerialDenseMatrix & *jacobianUX*) [static, private]

Jacobian of mapping from u to x random variable space.

This procedure computes the jacobian of the transformation from u to x space.

uncorr_normal_vars is the vector of random variables in standard normal space (u-space).

random_vars is the vector of the random variables in the user-defined x-space

6.61.2.12 void NonDAdvMeanValue::transNataf (Epetra_SerialSymDenseMatrix & *mod_corr_matrix*) [static, private]

This procedure modifys the correlation matrix input by the user to be used in the Nataf distribution model.

This procedure modifys the correlation matrix input by the user to be used in the Nataf distribution model (der Kiureghian and Liu, ASCE JEM 112:1, 1986).

R: the correlation coefficient matrix of the random variables

mod_corr_matrix: modified correlation matrix

Note: The modification is exact for log-log,normal-log,normal-normal, normal-uniform tranformations (numerical precision)

The uniform-uniform and uniform-log case are approximations obtained in the above reference.

6.61.3 Member Data Documentation

6.61.3.1 Epetra_SerialDenseVector NonDAdvMeanValue::correctedRespLevel [static, private]

output response levels calculated.

identical to responseLevelTargets for AMV+, FORM but will differ for AMV

The documentation for this class was generated from the following files:

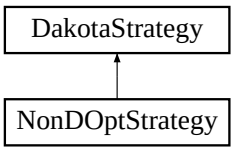
- NonDAdvMeanValue.H
- NonDAdvMeanValue.C

6.62 NonDOptStrategy Class Reference

Strategy for optimization under uncertainty (robust and reliability-based design).

`#include <NonDOptStrategy.H>`

Inheritance diagram for NonDOptStrategy::



Public Methods

- NonDOptStrategy (ProblemDescDB &problem_db)

  constructor.

- ~NonDOptStrategy ()

  destructor.

- void run_strategy ()

  Perform the strategy by executing optIterator (an optimizer) on designModel (a layered or nested model containing a nondeterministic iterator at a lower level).

Private Attributes

- DakotaModel designModel

  the nested or layered model interfaced with optIterator.

- DakotaIterator optIterator

  the top level optimizer.

6.62.1 Detailed Description

Strategy for optimization under uncertainty (robust and reliability-based design).

This strategy uses a NestedModel to nest an uncertainty quantification iterator within an optimization iterator in order to perform optimization using nondeterministic data. For OUU based on surrogates, LayeredModels are also employed, and the general recursion facilities supported by nested and layered models allow a broad array of OUU formulations. This class is very simple and is essentially identical to SingleMethodStrategy since all of the nested iteration mappings are contained within NestedModel::response_mapping().

The documentation for this class was generated from the following files:

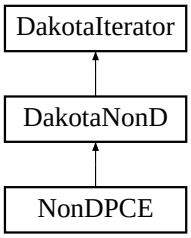
- NonDOptStrategy.H
- NonDOptStrategy.C

6.63 NonDPCE Class Reference

Stochastic finite element approach to uncertainty quantification using polynomial chaos expansions.

`#include <NonDPCE.H>`

Inheritance diagram for NonDPCE::



Public Methods

- NonDPCE (DakotaModel &model)

  constructor.

- ~NonDPCE ()

  destructor.

- void quantify_uncertainty ()

  virtual function to perform uncertainty quantification using SFEM/PCE methods outputs coefficients of polynomial chaos expansions.

- void print_iterator_results (ostream &s) const

  print the final statistics and PCE coefficient array.

Static Public Attributes

- DakotaRealVectorArray coeffArray

  Array containing Polynomial Chaos coefficients.

Private Methods

- void run_lhs ()

  generates the desired set of parameter samples from within user-specified probabilistic distributions.

Private Attributes

- LatinHypercube * lhsSampler

  pointer to the LatinHypercube object (responsible for generating the parameter samples).

- DakotaRealVectorArray paramSamples

  the set of parameter samples output from LHS. The double array from Fortran (arranged head to tail by parameter: all observations for var 1 followed by all observations for var 2, etc.) is converted to this array of DakotaRealVectors.*

- DakotaRealVectorArray responseFnSamples

  the response data (fn values only) for the parameter samples arranged as an array of DakotaRealVectors. This parallels paramSamples so that either may be used in vector_statistics().

- int numObservations

  the number of samples.

- int randomSeed

  the random number seed.

- DakotaString sampleType

  the sample type: "lhs" or "random".

- DakotaRealArray respThresh

  response thresholds for computing failure probabilities.

- short statsFlag

  flags computation/output of statistics.

- short allDataFlag

  flags update of allVariables/allResponses.

- size_t numActiveVars

  total number of variables published to LHS.

- int numX

  Number of Xi's in Polynomial Chaos Expansion.

- int highestOrder

  Highest order of Hermite Polynomials in Expansion.

- int numChaos

  Number of terms in Polynomial Chaos Expansion.

6.63.1 Detailed Description

Stochastic finite element approach to uncertainty quantification using polynomial chaos expansions.

The NonDPCE class uses a polynomial chaos expansion (PCE) approach to approximate the effect of parameter uncertainties on response functions of interest. It utilizes the HermiteSurf and HermiteChaos classes to perform the PCE.

The documentation for this class was generated from the following files:

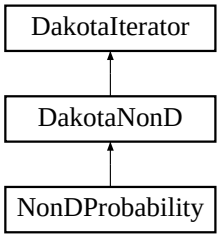
- NonDPCE.H
- NonDPCE.C

6.64 NonDProbability Class Reference

Wrapper class for the LHS library.

`#include <NonDProbability.H>`

Inheritance diagram for NonDProbability::



Public Methods

- NonDProbability (DakotaModel &model)

  constructor.

- NonDProbability (DakotaModel &model, int samples, int seed, const DakotaString &sampling_method, const short &opt_flag)

  alternate constructor for instantiations "on the fly".

- ~NonDProbability ()

  destructor.

- void quantify_uncertainty ()

  performs a forward uncertainty propagation by using LHS to generate a set of parameter samples, performing function evaluations on these parameter samples, and computing statistics on the ensemble of results.

- void print_iterator_results (ostream &s) const

  print the final statistics.

- void sampling_reset (int min_samples, short all_data_flag, short stats_flag)

  resets number of samples and sampling flags.

- const DakotaString & sampling_scheme () const

  return sampleType: "lhs" or "random".

Private Methods

- void run_lhs ()

  generates the desired set of parameter samples from within user-specified probabilistic distributions.

Private Attributes

- LatinHypercube * lhsSampler

  pointer to the LatinHypercube object (responsible for generating the parameter samples).

- DakotaRealVectorArray paramSamples

  the set of parameter samples output from LHS. The double array from Fortran (arranged head to tail by parameter: all observations for var 1 followed by all observations for var 2, etc.) is converted to this array of DakotaRealVectors.*

- DakotaRealVectorArray responseFnSamples

  the response data (fn values only) for the parameter samples arranged as an array of DakotaRealVectors. This parallels paramSamples so that either may be used in vector_statistics().

- int numObservations

  the number of samples to evaluate.

- int randomSeed

  the random number seed.

- DakotaString sampleType

  the sample type: "lhs" or "random".

- DakotaRealArray respThresh

  response thresholds for computing failure probabilities.

- short allVarsFlag

  flags DACE mode using all variables.

- short statsFlag

  flags computation/output of statistics.

- short allDataFlag

  flags update of allVariables/allResponses.

- size_t numActiveVars

  total number of variables published to LHS.

- size_t numDesignVars

  number of design variables (treated as uniform distribution within design variable bounds for DACE usage of NonDProbability).

- size_t numStateVars

  number of state variables (treated as uniform distribution within state variable bounds for DACE usage of NonDProbability).

6.64.1 Detailed Description

Wrapper class for the LHS library.

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 correlations through use of a mixing routine. The NonDProbability class provides a C++ wrapper for the LHS library and is used for performing forward propagations of parameter uncertainties into response statistics. The current LHS version in use dates back to a 1970's vintage Fortran version that was converted to C using f2c and then recast as C++ classes. These classes appear in the LatinHypercube (main LHS class which generates a set of samples from parameter distributions), LHSInput (random variable and user input classes), and LHSVecMatUtil (vector/matrix utilities) files. These files are undocumented as this version is due to be replaced with the 1998 Fortran LHS version shortly.

6.64.2 Constructor & Destructor Documentation

6.64.2.1 NonDProbability::NonDProbability (DakotaModel & *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.

6.64.2.2 NonDProbability::NonDProbability (DakotaModel & *model*, int *samples*, int *seed*, const DakotaString & *sampling_method*, const short & *opt_flag*)

alternate constructor for instantiations "on the fly".

This alternate constructor (currently inactive) is used by ApproximationInterface for uniform sampling. It is _not_ a letter-envelope instantiation and a set_db_list_nodes has not been performed. It is called with data from the approximation interface specification (not the method specification) passed through the constructor. This works because NoDBBaseConstructor is used and all of the relevant data for this NonDProbability usage can be taken from the incoming model. Thus, the following attributes are not initialized and should not be used: maxIterations, maxFunctionEvals, verboseOutput, methodName.

6.64.3 Member Function Documentation

6.64.3.1 void NonDProbability::quantify_uncertainty () [virtual]

performs a forward uncertainty propagation by using LHS to generate a set of parameter samples, performing function evaluations on these parameter samples, and computing statistics on the ensemble of results.

Loop over set of samples and compute responses. paramSamples contains an array ordered with all observations for parameter 1 followed by all observations for parameter 2, etc. After each response is computed, the value returned in current_response is compared to the threshold value, respThresh. The counter, less_than_thresh, is then incremented if the returned value is < respThresh.

Reimplemented from DakotaNonD.

6.64.3.2 void NonDProbability::sampling_reset (int *min_samples*, short *all_data_flag*, short *stats_flag*) [inline, virtual]

resets number of samples and sampling flags.

used by ApproximationInterface::build_global_approximation() 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 DakotaIterator.

The documentation for this class was generated from the following files:

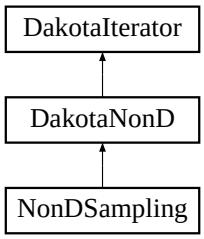
- NonDProbability.H
- NonDProbability.C

6.65 NonDSampling Class Reference

Wrapper class for the Fortran 90 LHS library.

`#include <NonDSampling.H>`

Inheritance diagram for NonDSampling::



Public Methods

- NonDSampling (DakotaModel &model)

  constructor.

- NonDSampling (DakotaModel &model, int samples, int seed, const DakotaString &sampling_method, const short &opt_flag)

  alternate constructor for instantiations "on the fly".

- ~NonDSampling ()

  destructor.

- void quantify_uncertainty ()

  performs a forward uncertainty propagation by using LHS to generate a set of parameter samples, performing function evaluations on these parameter samples, and computing statistics on the ensemble of results.

- void print_iterator_results (ostream &s) const

  print the final statistics.

- void sampling_reset (int min_samples, short all_data_flag, short stats_flag)

  resets number of samples and sampling flags.

- const DakotaString & sampling_scheme () const

  return sampleType: "lhs" or "random".

Private Methods

- void run_lhs ()

  generates the desired set of parameter samples from within user-specified probabilistic distributions.

- void check_error (const int &err_code, const char *err_source) const

  checks the return codes from LHS routines and aborts if an error is returned.

Private Attributes

- DakotaRealVectorArray paramSamples

  the set of parameter samples output from LHS. The double array from Fortran (arranged head to tail by parameter: all observations for var 1 followed by all observations for var 2, etc.) is converted to this array of DakotaRealVectors.*

- DakotaRealVectorArray responseFnSamples

  the response data (fn values only) for the parameter samples arranged as an array of DakotaRealVectors. This parallels paramSamples so that either may be used in vector_statistics().

- int numObservations

  the number of samples to evaluate.

- int randomSeed

  the random number seed.

- DakotaString sampleType

  the sample type: "lhs" or "random".

- DakotaRealArray respThresh

  response thresholds for computing failure probabilities.

- short allVarsFlag

  flags DACE mode using all variables.

- short statsFlag

  flags computation/output of statistics.

- short allDataFlag

  flags update of allVariables/allResponses.

- size_t numActiveVars

  total number of variables published to LHS.

- size_t numDesignVars

  number of design variables (treated as uniform distribution within design variable bounds for DACE usage of NonDSampling).

- size_t numStateVars

  number of state variables (treated as uniform distribution within state variable bounds for DACE usage of NonDSampling).

6.65.1 Detailed Description

Wrapper class for the Fortran 90 LHS library.

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 NonDSampling class provides a C++ wrapper for the LHS library and is used for performing forward propagations of parameter uncertainties into response statistics. The current LHS version reflects the 1998 Fortran 90 LHS version (as documented in SAND98-0210), which was converted to a UNIX link library in 2001. Thus, the NonDSampling class supercedes NonDProbability, which used a 1970's vintage LHS that had been f2c'd and converted to (incomplete) classes.

6.65.2 Constructor & Destructor Documentation

6.65.2.1 NonDSampling::NonDSampling (DakotaModel & *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.

6.65.2.2 NonDSampling::NonDSampling (DakotaModel & *model*, int *samples*, int *seed*, const DakotaString & *sampling_method*, const short & *opt_flag*)

alternate constructor for instantiations "on the fly".

This alternate constructor (currently inactive) is used by ApproximationInterface for uniform sampling. It is _not_ a letter-envelope instantiation and a set_db_list_nodes has not been performed. It is called with data from the approximation interface specification (not the method specification) passed through the constructor. This works because NoDBBaseConstructor is used and all of the relevant data for this NonDSampling usage can be taken from the incoming model. Thus, the following attributes are not initialized and should not be used: maxIterations, maxFunctionEvals, verboseOutput, methodName.

6.65.3 Member Function Documentation

6.65.3.1 void NonDSampling::quantify_uncertainty () [virtual]

performs a forward uncertainty propagation by using LHS to generate a set of parameter samples, performing function evaluations on these parameter samples, and computing statistics on the ensemble of results.

Loop over set of samples and compute responses. paramSamples contains an array ordered with all observations for parameter 1 followed by all observations for parameter 2, etc. After each response is computed, the value returned in current_response is compared to the threshold value, respThresh. The counter, less_than_thresh, is then incremented if the returned value is < respThresh.

Reimplemented from DakotaNonD.

6.65.3.2 void NonDSampling::sampling_reset (int *min_samples*, short *all_data_flag*, short *stats_flag*) [inline, virtual]

resets number of samples and sampling flags.

used by ApproximationInterface::build_global_approximation() 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 DakotaIterator.

The documentation for this class was generated from the following files:

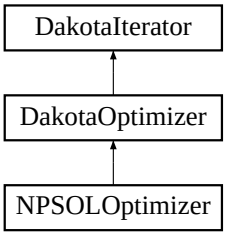
- NonDSampling.H
- NonDSampling.C

6.66 NPSOLOptimizer Class Reference

Wrapper class for the NPSOL optimization library.

`#include <NPSOLOptimizer.H>`

Inheritance diagram for NPSOLOptimizer::



Public Methods

- NPSOLOptimizer (DakotaModel &model)

  standard constructor.

- NPSOLOptimizer (const DakotaRealVector &initial_point, const DakotaRealVector &var_lower_bnds, const DakotaRealVector &var_upper_bnds, int num_lin_ineq, int num_lin_eq, int num_nln_ineq, int num_nln_eq, const DakotaRealMatrix &lin_ineq_coeffs, const DakotaRealVector &lin_ineq_lower_bnds, const DakotaRealVector &lin_ineq_upper_bnds, const DakotaRealMatrix &lin_eq_coeffs, const DakotaRealVector &lin_eq_targets, const DakotaRealVector &nonlin_ineq_lower_bnds, const DakotaRealVector &nonlin_ineq_upper_bnds, const DakotaRealVector &nonlin_eq_targets, void(*user_obj_eval)(int &, int &, Real *, Real &, Real *, int &), void(*user_con_eval)(int &, int &, int &, int &, int *, Real *, Real *, Real *, int &), int derivative_level)

  special constructor for instantiations "on the fly".

- ~NPSOLOptimizer ()

  destructor.

- void find_optimum ()

  Used within the optimizer branch for computing the optimal solution. Redefines the run_iterator virtual function for the optimizer branch.

Private Methods

- void find_optimum_on_model ()

  called by find_optimum for setUpType == "model".

- void find_optimum_on_user_functions ()

  called by find_optimum for setUpType == "user_functions".

- void allocate_workspace ()

  Allocates workspace for the optimizer. Private method for the NPSOLOptimizer constructors.

- void augment_bounds (DakotaRealVector &augmented_lower_bnds, DakotaRealVector &augmented_upper_bnds)

  augments variable bounds with linear and nonlinear constraint bounds.

Static Private Methods

- void objective_f_eval (int &mode, int &num_parameters, Real *x, Real &f, Real *g, int &state)

  OBJFUN in NPSOL manual: computes the value and first derivatives of the objective function (passed by function pointer to NPSOL).

- void constraint_f_eval (int &mode, int &ncnln, int &n, int &nrowj, int *needc, Real *x, Real *c, Real *cjac, int &nstate)

  CONFUN in NPSOL manual: computes the values and first derivatives of the nonlinear constraint functions (passed by function pointer to NPSOL).

Private Attributes

- int linConstraintMatrixSize

  used for non-zero array sizing (linear constraints).

- DakotaRealArray cLambda

  CLAMBDA from NPSOL manual: Langrange multipliers.

- DakotaIntArray 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 augmented 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.

- DakotaString setUpType

  controls iteration mode: "model" (normal usage) or "user_functions" (user-supplied functions mode for "on the fly" instantiations). NonDAdvMeanValue currently uses the user_functions mode.

- DakotaRealVector initialPoint

  holds initial point passed in for "user_functions" mode.

- DakotaRealVector lowerBounds

  holds variable lower bounds passed in for "user_functions" mode.

- DakotaRealVector upperBounds

  holds variable upper bounds passed in for "user_functions" mode.

- void(* userObjectiveEval)(int &, int &, Real *, Real &, Real *, int &)

  holds function pointer for objective function evaluator passed in for "user_functions" mode.

- void(* userConstraintEval)(int &, int &, int &, int &, int *, Real *, Real *, Real *, int &)

  holds function pointer for constraint function evaluator passed in for "user_functions" mode.

Static Private Attributes

- int fnEvalCntr

  counter for testing against staticMaxFnEvals.

- int staticMaxFnEvals

  static copy of DakotaIterator::maxFunctionEvals.

- int staticVendorNumericalGradFlag

  static copy of DakotaOptimizer::vendorNumericalGradFlag.

6.66.1 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 static as well. To isolate the effect of these static requirements from the rest of the iterator hierarchy, static copies are made of many non-static attributes inherited from above.

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 npoptn_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.

The documentation for this class was generated from the following files:

- NPSOLOptimizer.H
- NPSOLOptimizer.C

6.67 ParallelLibrary Class Reference

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

`#include <ParallelLibrary.H>`

Public Methods

- ParallelLibrary (int &argc, char **&argv)
  constructor.
- ParallelLibrary ()
  default constructor (used only for dummy_lib).
- ~ParallelLibrary ()
  destructor.
- void init_iterator_communicators (const ProblemDescDB &problem_db)
  split MPI_COMM_WORLD into iterator communicators.
- void init_evaluation_communicators (int eval_servers, int procs_per_eval, int max_concurrency, int asynch_local_eval_concurrency, const DakotaString &eval_scheduling)
  split an iterator communicator into evaluation communicators.
- void init_analysis_communicators (int analysis_servers, int procs_per_analysis, int max_concurrency, int asynch_local_analysis_concurrency, const DakotaString &analysis_scheduling)
  split an evaluation communicator into analysis communicators.
- void free_iterator_communicators ()
  deallocate iterator communicators.
- void free_evaluation_communicators ()
  deallocate evaluation communicators.
- void free_analysis_communicators ()
  deallocate analysis communicators.
- void print_configuration ()
  print the parallel configuration for all parallelism levels.
- void send_si (PackBuffer &send_buffer, int dest, int tag)
  blocking send at the strategy-iterator communication level.
- void isend_si (PackBuffer &send_buffer, int dest, int tag, MPI_Request &send_request)
  nonblocking send at the strategy-iterator communication level.
- void recv_si (UnPackBuffer &recv_buffer, int source, int tag, MPI_Status &status)

blocking receive at the strategy-iterator communication level.

- void irecv_si (UnPackBuffer &recv_buffer, int source, int tag, MPI_Request &recv_request)
  nonblocking receive at the strategy-iterator communication level.
- void send_ie (PackBuffer &send_buffer, int dest, int tag)
  blocking send at the iterator-evaluation communication level.
- void isend_ie (PackBuffer &send_buffer, int dest, int tag, MPI_Request &send_request)
  nonblocking send at the iterator-evaluation communication level.
- void recv_ie (UnPackBuffer &recv_buffer, int source, int tag, MPI_Status &status)
  blocking receive at the iterator-evaluation communication level.
- void irecv_ie (UnPackBuffer &recv_buffer, int source, int tag, MPI_Request &recv_request)
  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_request)
  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_request)
  nonblocking receive at the evaluation-analysis communication level.
- void bcast (int &data, MPI_Comm comm)
  broadcast an integer across a communicator.
- void bcast (PackBuffer &send_buffer, MPI_Comm comm)
  send a packed buffer across a communicator using a broadcast.
- void bcast (UnPackBuffer &recv_buffer, MPI_Comm comm)
  matching receive for a packed buffer broadcast.
- void waitall (int num_recvs, MPI_Request *&recv_requests)
  wait for all messages from a series of nonblocking receives.
- int world_size () const
  return worldSize.
- int world_rank () const
  return worldRank.
- short parallelism_levels () const
  return parallelismLevels.

- short strategy_dedicated_master_flag () const
  return strategyDedicatedMasterFlag.
- short strategy_iterator_split_flag () const
  return stratIteratorSplitFlag.
- short iterator_master_flag () const
  return iteratorMasterFlag.
- short strategy_iterator_message_pass () const
  return stratIteratorMessagePass.
- MPI_Comm iterator_intra_communicator () const
  return iteratorIntraComm.
- MPI_Comm strategy_iterator_inter_communicator () const
  return stratIteratorInterComm.
- MPI_Comm * strategy_iterator_inter_communicators () const
  return stratIteratorInterComms.
- int iterator_servers () const
  return numIteratorServers.
- int iterator_communicator_rank () const
  return iteratorCommRank.
- int iterator_communicator_size () const
  return iteratorCommSize.
- int iterator_server_id () const
  return iteratorServerId.
- short iterator_dedicated_master_flag () const
  return iteratorDedicatedMasterFlag.
- short iterator_eval_split_flag () const
  return iteratorEvalSplitFlag.
- short evaluation_master_flag () const
  return evalMasterFlag.
- short iterator_eval_message_pass () const
  return iteratorEvalMessagePass.
- MPI_Comm evaluation_intra_communicator () const
  return evalIntraComm.
- MPI_Comm iterator_eval_inter_communicator () const
  return iteratorEvalInterComm.

- MPI_Comm * iterator_eval_inter_communicators () const
  return iteratorEvalInterComms.
- int evaluation_servers () const
  return numEvalServers.
- int evaluation_communicator_rank () const
  return evalCommRank.
- int evaluation_communicator_size () const
  return evalCommSize.
- int evaluation_server_id () const
  return evalServerId.
- short evaluation_dedicated_master_flag () const
  return evalDedicatedMasterFlag.
- short eval_analysis_split_flag () const
  return evalAnalysisSplitFlag.
- short analysis_master_flag () const
  return analysisMasterFlag.
- short eval_analysis_message_pass () const
  return evalAnalysisMessagePass.
- MPI_Comm analysis_intra_communicator () const
  return analysisIntraComm.
- MPI_Comm eval_analysis_inter_communicator () const
  return evalAnalysisInterComm.
- MPI_Comm * eval_analysis_inter_communicators () const
  return evalAnalysisInterComms.
- int analysis_servers () const
  return numAnalysisServers.
- int analysis_communicator_rank () const
  return analysisCommRank.
- int analysis_communicator_size () const
  return analysisCommSize.
- int analysis_server_id () const
  return analysisServerId.

Private Methods

- short split_communicator_dedicated_master (MPI_Comm parent_comm, const int &parent_comm_rank, const int &parent_comm_size, const int &num_servers, const int &procs_per_server, const int &proc_remainder, MPI_Comm &child_intra_comm, int &child_comm_rank, int &child_comm_size, MPI_Comm &child_inter_comm, MPI_Comm *&child_inter_comms, int &server_id, short &child_master_flag)

  split a parent communicator into a dedicated master processor and num_servers child communicators.

- short split_communicator_peer_partition (MPI_Comm parent_comm, const int &parent_comm_rank, const int &parent_comm_size, const int &num_servers, const int &procs_per_server, const int &proc_remainder, MPI_Comm &child_intra_comm, int &child_comm_rank, int &child_comm_size, MPI_Comm &child_inter_comm, MPI_Comm *&child_inter_comms, int &peer_id, short &child_master_flag)

  split a parent communicator into num_servers child communicators (no dedicated master processor).

- short resolve_inputs (int &num_servers, int &procs_per_server, const int &avail_procs, int &proc_remainder, const int &max_concurrency, const int &capacity_multiplier, const DakotaString &default_config, const DakotaString &scheduling_override)

  Resolve user inputs into a sensible partitioning scheme.

Private Attributes

- int worldSize

  size of MPI_COMM_WORLD.

- int worldRank

  rank in MPI_COMM_WORLD.

- short parallelismLevels

  number of parallelism levels.

- short mpirunFlag

  flag for a parallel mpirun/yod launch.

- short dummyFlag

  prevents multiple MPI_Finalize calls due to dummy_lib.

- 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.

- short strategyDedicatedMasterFlag
  signals ded. master partitioning.
- short stratIteratorSplitFlag
  signals a communicator split was used.
- short iteratorMasterFlag
  identifies master iterator processors.
- short stratIteratorMessagePass
  flag for message passing at si level.
- MPI_Comm iteratorIntraComm
  intracomm for each iterator partition.
- MPI_Comm stratIteratorInterComm
  intercomm between an iterator & master strategy (on iterator partitions only).
- MPI_Comm * stratIteratorInterComms
  intercomm. array on master strategy.
- int numIteratorServers
  number of iterator servers.
- int procsPerIterator
  processors per iterator server.
- int iteratorCommRank
  rank in iteratorIntraComm.
- int iteratorCommSize
  size of iteratorIntraComm.
- int iteratorServerId
  identifier for an iterator server.
- short iteratorDedicatedMasterFlag
  signals ded. master partitioning.
- short iteratorEvalSplitFlag
  signals a communicator split was used.
- short evalMasterFlag
  identifies master evaluation processors.
- short iteratorEvalMessagePass
  flag for message passing at ie level.
- MPI_Comm evalIntraComm

intracomm for each fn. eval. partition.

- MPI_Comm iteratorEvalInterComm
  intercomm between a fn. eval. & master iterator (on fn. eval. partitions only).
- MPI_Comm * iteratorEvalInterComms
  intercomm array on master iterator.
- int numEvalServers
  number of evaluation servers.
- int procsPerEval
  processors per evaluation server.
- int evalCommRank
  rank in evalIntraComm.
- int evalCommSize
  size of evalIntraComm.
- int evalServerId
  identifier for an evaluation server.
- short evalDedicatedMasterFlag
  signals dedicated master partitioning.
- short evalAnalysisSplitFlag
  signals a communicator split was used.
- short analysisMasterFlag
  identifies master analysis processors.
- short evalAnalysisMessagePass
  flag for message passing at ea level.
- MPI_Comm analysisIntraComm
  intracomm for each analysis partition.
- MPI_Comm evalAnalysisInterComm
  intercomm between an analysis & master fn. eval. (on analysis partitions only).
- MPI_Comm * evalAnalysisInterComms
  intercomm array on master fn. eval.
- int numAnalysisServers
  number of analysis servers.
- int procsPerAnalysis
  processors per analysis server.

- int analysisCommRank

  rank in analysisIntraComm.

- int analysisCommSize

  size of analysisIntraComm.

- int analysisServerId

  identifier for an analysis server.

6.67.1 Detailed Description

Class for managing partitioning of multiple levels of parallelism and message passing within the 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, then ParallelLibrary should become a class hierarchy with virtual functions to encapsulate the library-specific syntax.

6.67.2 Member Function Documentation

6.67.2.1 void ParallelLibrary::init_iterator_communicators (const ProblemDescDB & *problem_db*)

split MPI_COMM_WORLD into iterator communicators.

Split MPI_COMM_WORLD into the specified number of subcommunicators to set up concurrent iterator partitions serving a strategy. This constructs new iterator intra-communicators and strategy-iterator inter-communicators. The init_iterator_communicators() and free_iterator_communicators() functions are both called from main.C, and init_iterator_communicators() is called prior to output and restart management since output and restart files are tagged based on iterator server id.

6.67.2.2 void ParallelLibrary::init_evaluation_communicators (int *eval_servers*, int *procs_per_eval*, int *max_concurrency*, int *asynch_local_eval_concurrency*, const DakotaString & *eval_scheduling*)

split an iterator communicator into evaluation communicators.

Split iteratorIntraComm (=MPI_COMM_WORLD if no concurrence in iterators) as specified by the passed parameters to set up concurrent evaluation partitions serving an iterator. This constructs new evaluation intra-communicators and iterator-evaluation inter-communicators. init_evaluation_communicators() is called from ApplicationInterface::init_communicators() and free_evaluation_communicators() function is called from ApplicationInterface::free_communicators(). eval_servers, asynch_local_eval_concurrency, and eval_scheduling come from the interface keyword specification. procs_per_eval is not directly user-specified, rather it contains the minimum procs_per_eval required to support any lower level user requests (such as procs_per_analysis). max_concurrency is passed in via the function DakotaIterator::max_concurrency(), which queries individual methods for their gradient configuration, population size, etc. These partitions can be reconfigured for each iterator/model pair within a strategy (e.g. interface 1 uses 4 by 256 while interface 2 uses 2 by 512) – see DakotaStrategy::run_iterator().

6.67.2.3 void ParallelLibrary::init_analysis_communicators (int *analysis_servers*, int *procs_per_analysis*, int *max_concurrency*, int *asynch_local_analysis_concurrency*, const DakotaString & *analysis_scheduling*)

split an evaluation communicator into analysis communicators.

Split evalIntraComm as indicated by the passed parameters to set up concurrent analysis partitions serving a function evaluation. This constructs new analysis intra-communicators and evaluation-analysis inter-communicators. init_analysis_communicators() is called from ApplicationInterface::init_communicators() following the call to init_evaluation_communicators() and free_analysis_communicators() is called from ApplicationInterface::free_communicators() preceding the call to free_evaluation_communicators(). The analysis_servers, procs_per_analysis, asynch_local_analysis_concurrency, and analysis_scheduling attributes come from the interface keyword specification, and max_concurrency contains the length of analysis_drivers from the interface keyword specification. The analysis partitions can be reconfigured for each iterator/model pair within a strategy.

6.67.2.4 short ParallelLibrary::resolve_inputs (int & *num_servers*, int & *procs_per_server*, const int & *avail_procs*, int & *proc_remainder*, const int & *max_concurrency*, const int & *capacity_multiplier*, const DakotaString & *default_config*, const DakotaString & *scheduling_override*) [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.

The documentation for this class was generated from the following files:

- ParallelLibrary.H
- ParallelLibrary.C

6.68 ParamResponsePair Class Reference

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

`#include <ParamResponsePair.H>`

Public Methods

- ParamResponsePair ()
  default constructor.
- ParamResponsePair (const DakotaVariables &vars, const DakotaResponse &response)
  alternate constructor for temporaries.
- ParamResponsePair (const DakotaVariables &vars, const DakotaResponse &response, const int id)
  standard constructor for history uses.
- ParamResponsePair (const ParamResponsePair &pair)
  copy constructor.
- ~ParamResponsePair ()
  destructor.
- ParamResponsePair & operator= (const ParamResponsePair &pair)
  assignment operator.
- void read (istream &s)
  read a ParamResponsePair object from an istream.
- void write (ostream &s) const
  write a ParamResponsePair object to an ostream.
- void read_annotated (istream &s)
  read a ParamResponsePair object in annotated format from an istream.
- void write_annotated (ostream &s) const
  write a ParamResponsePair object in annotated format to an ostream.
- void write_tabular (ostream &s) const
  write a ParamResponsePair object in tabular format to an ostream.
- void read (DakotaBiStream &s)
  read a ParamResponsePair object from the binary restart stream.
- void write (DakotaBoStream &s) const
  write a ParamResponsePair object to the binary restart stream.

- void read (UnPackBuffer &s)

  read a ParamResponsePair object from a packed MPI buffer.

- void write (PackBuffer &s) const

  write a ParamResponsePair object to a packed MPI buffer.

- int eval_id () const

  return the evaluation identifier.

- const DakotaVariables & prp_parameters () const

  return the parameters object.

- const DakotaResponse & prp_response () const

  return the response object.

- void prp_response (const DakotaResponse &response)

  set the response object.

- const DakotaIntArray & active_set_vector () const

  return the active set vector from the response object.

- void active_set_vector (const DakotaIntArray &asv)

  set the active set vector in the response object.

- const DakotaString & interface_id () const

  return the interface identifier from the response object.

Private Attributes

- DakotaVariables prPairParameters

  the set of parameters for the function evaluation.

- DakotaResponse prPairResponse

  the response set for the function evaluation.

- int evalId

  the function evaluation identifier (assigned from ApplicationInterface::fnEvalId).

Friends

- int operator== (const ParamResponsePair &pair1, const ParamResponsePair &pair2)

  equality operator.

6.68.1 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 list, in restart file operations, and in a variety of scheduling algorithm bookkeeping operations. With the advent of STL, replacement of this class with the pair<> template construct may be possible (using pair<int, pair<vars,response> >, for example), assuming that deep copies, I/O, alternate constructors, etc., can be adequately addressed.

6.68.2 Constructor & Destructor Documentation

6.68.2.1 ParamResponsePair::ParamResponsePair (const DakotaVariables & *vars*, const DakotaResponse & *response*) [inline]

alternate constructor for temporaries.

This constructor can use the standard DakotaVariables and DakotaResponse copy constructors to share representations since this constructor is 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).

6.68.2.2 ParamResponsePair::ParamResponsePair (const DakotaVariables & *vars*, const DakotaResponse & *response*, const int *id*) [inline]

standard constructor for history uses.

This constructor cannot share representations since it involves a history mechanism (beforeSynchPRPList or data_pairs). Deep copies must be made.

6.68.3 Member Data Documentation

6.68.3.1 int ParamResponsePair::evalId [private]

the function evaluation identifier (assigned from ApplicationInterface::fnEvalId).

evalId belongs here rather than in DakotaResponse since some DakotaResponse objects involve consolidation of several fn. evals. (e.g., synchronize_fd_gradients). The prPair, on the other hand, is used for storage of all low level fn. evals. that get evaluated, so evalId is meaningful.

The documentation for this class was generated from the following files:

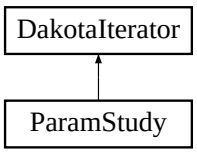
- ParamResponsePair.H
- ParamResponsePair.C

6.69 ParamStudy Class Reference

Class for vector, list, centered, and multidimensional parameter studies.

`#include <ParamStudy.H>`

Inheritance diagram for ParamStudy::



Public Methods

- ParamStudy (DakotaModel &model)
  constructor.
- ~ParamStudy ()
  destructor.
- void run_iterator ()
  run the iterator.
- const DakotaVariables & iterator_variable_results () const
  return the final iterator solution (variables).
- const DakotaResponse & iterator_response_results () const
  return the final iterator solution (response).
- void print_iterator_results (ostream &s) const
  print the final iterator results.

Private Methods

- void compute_vector_steps ()
  computes stepVector and numSteps from initialPoint, finalPoint, and either numSteps or stepLength (pStudyType is 1 or 2).
- void vector_loop (const DakotaRealVector &start, const DakotaRealVector &step_vect, const int &num_steps)
  performs the parameter study by looping from start in num_steps increments of step_vect. Total number of evaluations is num_steps + 1.
- void sample (const DakotaRealVector &list_of_points)

performs the parameter study by sampling from a list of points.

- void centered_loop (const DakotaRealVector &start, const Real &percent_delta, const int &deltas_per_variable)

  performs a number of plus and minus offsets for each parameter centered about start.

- void multidim_loop (const DakotaIntArray &var_partitions)

  performs vector_loops recursively in multiple dimensions.

- void recurse (int nloop, int nindex, DakotaIntArray &current_index, const DakotaIntArray &max_index, const DakotaRealVector &start, const DakotaRealVector &step_vect)

  used by multidim_loop to enable a variable number of nested loops.

- void update_best (const DakotaRealVector &vars, const DakotaResponse &response, const int eval_num)

  compares current evaluation to best evaluation and updates best.

Private Attributes

- DakotaRealVector listOfPoints

  list of evaluation points for the list_parameter_study.

- DakotaRealVector initialPoint

  the starting point for vector and centered parameter studies.

- DakotaRealVector finalPoint

  the ending point for vector_parameter_study (a specification option).

- DakotaRealVector stepVector

  the n-dimensional increment in vector_parameter_study.

- int numSteps

  the number of times stepVector is applied in vector_parameter_study.

- int pStudyType

  internal code for parameter study type: -1 (list), 1,2,3 (different vector specifications), 4 (centered), or 5 (multidim).

- int deltasPerVariable

  number of offsets in the plus and the minus direction for each variable in a centered_parameter_study.

- short nestedFlag

  flag set by parameter studies which call other parameter studies in loops.

- short recurseFlag

  flag set after initial loop in a nested study (so update_best() works with eval_num==0 multiple times).

- Real stepLength

  the Cartesian length of multidimensional steps in vector_parameter_study (a specification option).

- Real percentDelta

  size of relative offsets in percent for each variable in a centered_parameter_study.

- DakotaIntArray variablePartitions

  number of partitions for each variable in a multidim_parameter_study.

- DakotaVariables bestVariables

  best variables found during the study.

- DakotaResponse bestResponses

  best responses found during the study.

- Real bestObjectiveFn

  best objective function found during the study.

- Real bestViolations

  best constraint violations found during the study. In the current approach, constraint violation reduction takes strict precedence over objective function reduction.

- size_t numObjectiveFunctions

  number of objective functions. Used in update_best.

- size_t numNonlinearIneqConstraints

  number of nonlinear inequality constraints. Used in update_best.

- size_t numNonlinearEqConstraints

  number of nonlinear equality constraints. Used in update_best.

- DakotaRealVector multiObjWeights

  vector of multiobjective weights. Used in update_best.

- DakotaRealVector nonlinearIneqLowerBnds

  vector of nonlinear inequality constraint lower bounds. Used in update_best.

- DakotaRealVector nonlinearIneqUpperBnds

  vector of nonlinear inequality constraint upper bounds. Used in update_best.

- DakotaRealVector nonlinearEqTargets

  vector of nonlinear equality constraint targets. Used in update_best.

- DakotaRealVectorArray vectorOfVars

  history of variable sets. Allows use of update_best in asynchronous mode. Needs class scope for nested parameter studies.

- int psCounter

  class-scope counter (needed for asynchronous multidim_loop).

6.69.1 Detailed Description

Class for vector, list, centered, and multidimensional parameter studies.

The ParamStudy class contains several algorithms for performing parameter studies of different types. It is not a wrapper for an external library, rather its algorithms are self-contained. 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 a specified number of intervals for each dimension. It is a nested study in that it utilizes the vector parameter study internally as it recurses through the variables. 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.

6.69.2 Member Function Documentation

6.69.2.1 void ParamStudy::run_iterator () [virtual]

run the iterator.

This function is the primary run function for the iterator class hierarchy. All derived classes need to redefine it.

Reimplemented from DakotaIterator.

The documentation for this class was generated from the following files:

- ParamStudy.H
- ParamStudy.C

6.70 ProblemDescDB Class Reference

The database containing information parsed from the DAKOTA input file.

`#include <ProblemDescDB.H>`

Public Methods

- ProblemDescDB (ParallelLibrary &parallel_lib)

  constructor.

- ~ProblemDescDB ()

  destructor.

- void check_input ()

  verifies that there was at least one of each of the required keywords in the dakota input file.

- void set_db_list_nodes (const DakotaString &method_tag)

  set methodIndex based on the method identifier string to activate a particular method specification in methodList and use pointers from this method specification to set the other list indices.

- void set_db_list_nodes (const int &method_index)

  set methodIndex to activate a particular method specification in methodList and use pointers from this method specification to set the other list indices.

- int get_db_list_nodes () const

  return the current methodIndex.

- void set_db_interface_node (const DakotaString &interface_tag)

  set interfaceIndex based on the interface identifier string.

- void set_db_interface_node (const int &interface_index)

  set interfaceIndex.

- int get_db_interface_node () const

  return the current interfaceIndex.

- void set_db_responses_node (const DakotaString &responses_tag)

  set responsesIndex based on the responses identifier string.

- void set_db_model_type (const DakotaString &model_type)

  set the model type.

- void send_db_buffer ()

  MPI send of a large buffer containing strategy specification attributes and all the objects in interfaceList, variablesList, methodList, and responsesList.

- void receive_db_buffer ()

  MPI receive of a large buffer containing strategy specification attributes and all the objects in interfaceList, variablesList, methodList, and responsesList.

- ParallelLibrary & parallel_library () const

  return the parallelLib reference.

- const DakotaRealVector & get_drv (const DakotaString &entry_name) const

  get a DakotaRealVector out of the database based on an identifier string.

- const DakotaIntVector & get_div (const DakotaString &entry_name) const

  get a DakotaIntVector out of the database based on an identifier string.

- const DakotaRealArray & get_dra (const DakotaString &entry_name) const

  get a DakotaRealArray out of the database based on an identifier string.

- const DakotaIntArray & get_dia (const DakotaString &entry_name) const

  get a DakotaIntArray out of the database based on an identifier string.

- const DakotaRealMatrix & get_drm (const DakotaString &entry_name) const

  get a DakotaRealMatrix out of the database based on an identifier string.

- const DakotaIntList & get_dil (const DakotaString &entry_name) const

  get a DakotaIntList out of the database based on an identifier string.

- const DakotaStringArray & get_dsa (const DakotaString &entry_name) const

  get a DakotaStringArray out of the database based on an identifier string.

- const DakotaStringList & get_dsl (const DakotaString &entry_name) const

  get a DakotaStringList out of the database based on an identifier string.

- const DakotaString & get_string (const DakotaString &entry_name) const

  get a DakotaString out of the database based on an identifier string.

- const Real & get_real (const DakotaString &entry_name) const

  get a Real out of the database based on an identifier string.

- const int & get_int (const DakotaString &entry_name) const

  get an int out of the database based on an identifier string.

- const size_t & get_sizet (const DakotaString &entry_name) const

  get a size_t out of the database based on an identifier string.

- const short & get_short (const DakotaString &entry_name) const

  get a short out of the database based on an identifier string.

Static Public Methods

- void method_kwhandler (const struct FunctionData *parsed_data)

  method keyword handler called by IDR when a complete method specification is parsed.

- void variables_kwhandler (const struct FunctionData *parsed_data)

  variables keyword handler called by IDR when a complete variables specification is parsed.

- void interface_kwhandler (const struct FunctionData *parsed_data)

  interface keyword handler called by IDR when a complete interface specification is parsed.

- void responses_kwhandler (const struct FunctionData *parsed_data)

  responses keyword handler called by IDR when a complete responses specification is parsed.

- void strategy_kwhandler (const struct FunctionData *parsed_data)

  strategy keyword handler called by IDR when a complete strategy specification is parsed.

Private Methods

- void set_other_list_nodes (const int &world_rank, const int &verbose_flag)

  convenience function used by set_db_list_nodes(method_tag) and set_db_list_nodes(method_index) to set the other list indices once methodIndex is set (based on pointers from the method specification).

Static Private Methods

- void build_label (DakotaString &label, const DakotaString &root_label, size_t tag)

  create a label by appending tag to root_label.

- void build_labels (DakotaStringArray &label_array, const DakotaString &root_label)

  create an array of labels by tagging root_label with index in label_array. Uses build_label().

Private Attributes

- ParallelLibrary & parallelLib

  reference to the parallel_lib object passed from main.

Static Private Attributes

- DakotaString strategyType

  the strategy selection: multi_level, surrogate_based_opt, opt_under_uncertainty, branch_and_bound, multi_start, pareto_set, or single_method.

- short strategyGraphicsFlag

  flags use of graphics by the strategy (from the graphics specification in **StratIndControl***).*

- short strategyTabularDataFlag

  flags tabular data collection by the strategy (from the tabular_graphics_data specification in **StratIndControl***).*

- DakotaString strategyTabularDataFile

  the filename used for tabular data collection by the strategy (from the tabular_graphics_file specification in **StratIndControl***).*

- int strategyIteratorServers

  number of servers for concurrent iterator parallelism (from the iterator_servers specification in **StratIndControl***).*

- DakotaString strategyIteratorScheduling

  type of scheduling (self or static) used in concurrent iterator parallelism (from the iterator_self_scheduling and iterator_static_scheduling specifications in **StratIndControl***).*

- DakotaString strategyMethodPointer

  method identifier for the strategy (from the opt_method_pointer specifications in **StratSBO**, **StratOUU**, **StratBandB**, *and* **StratParetoSet** *and method_pointer specifications in* **StratSingle** *and* **StratMultiStart***).*

- int strategyBandBNumSamplesRoot

  number of samples at the root for the branch and bound strategy (from the num_samples_at_root specification in **StratBandB***).*

- int strategyBandBNumSamplesNode

  number of samples at each node for the branch and bound strategy (from the num_samples_at_node specification in **StratBandB***).*

- DakotaStringList strategyMultilevelMethodList

  list of methods for the multilevel hybrid optimization strategy (from the method_list specification in **StratML***).*

- DakotaString strategyMultilevelType

  the type of multilevel hybrid optimization strategy: uncoupled, uncoupled_adaptive, or coupled (from the uncoupled, adaptive, and coupled specifications in **StratML***).*

- Real strategyMultilevelProgThresh

  progress threshold for uncoupled_adaptive multilevel hybrids (from the progress_threshold specification in **StratML***).*

- DakotaString strategyMultilevelGlobalMethodPointer

  global method pointer for coupled multilevel hybrids (from the global_method_pointer specification in **StratML***).*

- DakotaString strategyMultilevelLocalMethodPointer

  local method pointer for coupled multilevel hybrids (from the local_method_pointer specification in **StratML***).*

- Real strategyMultilevelLSProb

  local search probability for coupled multilevel hybrids (from the local_search_probability specification in **StratML***).*

- int strategySBOMaxIterations

  maximum number of iterations in the surrogate-based optimization strategy (from the max_iterations specification in **StratSBO***).*

- Real strategySBOTRInitSize

  initial trust region size in the surrogate-based optimization strategy (from the initial_size specification in **StratSBO***).*

- Real strategySBOTRContract

  trust region contraction factor in the surrogate-based optimization strategy (from the contraction_factor specification in **StratSBO***).*

- Real strategySBOTRExpand

  trust region expansion factor in the surrogate-based optimization strategy (from the expansion_factor specification in **StratSBO***).*

- int strategyConcurrentNumJobs

  number of iterator jobs to perform in the concurrent strategy (from the num_starts and num_optima specifications in **StratMultiStart** *and* **StratParetoSet***).*

- DakotaRealVector strategyConcurrentParameterSets

  number of parameter sets to evaluate in the concurrent strategy (from the starting_points and multi_objective_weight_sets specifications in **StratMultiStart** *and* **StratParetoSet***).*

- DakotaList< DataMethod > methodList

  list of method specifications, one for each call to method_kwhandler by the parser.

- DakotaList< DataVariables > variablesList

  list of variables specifications, one for each call to variables_kwhandler by the parser.

- DakotaList< DataInterface > interfaceList

  list of interface specifications, one for each call to interface_kwhandler by the parser.

- DakotaList< DataResponses > responsesList

  list of responses specifications, one for each call to responses_kwhandler by the parser.

- int methodIndex

  index into methodList (identifies the active method specification).

- int variablesIndex

  index into variablesList (identifies the active variables specification).

- int interfaceIndex

  index into interfaceList (identifies the active interface specification).

- int responsesIndex

  index into responsesList (identifies the active responses specification).

- int strategyIndex

  used only in check_input (there is no strategy specification list) to verify that there is only one strategy specification.

6.70.1 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 the Input Deck Reader (IDR) parser. When the parser reads a complete keyword (delimited by a newline), it calls the corresponding kwhandler function from this class, which (for method, variables, interface, or responses specifications) populates a data class object (DataMethod, DataVariables, DataInterface, or DataResponses) and appends the object to a linked list (methodList, variablesList, interfaceList, or responsesList). The strategy_kwhandler is the exception to this, since the restriction of only allowing one strategy specification means there's no need for a DataStrategy class or a strategyList (instead, strategy attributes are members of ProblemDescDB). For information on modifying the input parsing procedures, refer to Dakota/docs/spec_change_instructions.txt

6.70.2 Member Function Documentation

6.70.2.1 void ProblemDescDB::set_db_model_type (const DakotaString & *model_type*)

set the model type.

Used to avoid recursion in DakotaModel::get_model() by a sub model when get_string("method.model_type") is not reset by a sub iterator. Note: if more needs of this type arise, could add set_<type> member functions to parallel the existing get_<type> member functions.

The documentation for this class was generated from the following files:

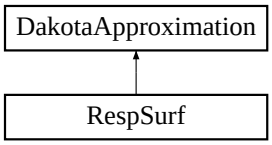
- ProblemDescDB.H
- ProblemDescDB.C

6.71 RespSurf Class Reference

Derived approximation class for quadratic polynomial regression.

`#include <RespSurf.H>`

Inheritance diagram for RespSurf::



Public Methods

- RespSurf (const ProblemDescDB &problem_db)

  constructor.

- ~RespSurf ()

  destructor.

Protected Methods

- void find_coefficients ()

  Least squares fit to data using a singular value decomposition.

- int required_samples (int num_vars)

  return the minimum number of samples required to build the derived class approximation type in num_vars dimensions.

- Real get_value (const DakotaRealVector &x)

  retrieve the approximate function value for a given parameter vector.

- const DakotaRealVector & get_gradient (const DakotaRealVector &x)

  retrieve the approximate function gradient for a given parameter vector.

Private Attributes

- int numRowsA

  Number of rows in matrix A.

- int numColsA

  Number of columns in matrix A.

- int numRHS

  Number of right hand side vectors for least squares solution.

- int leadDimA

  The leading dimension of matrix A.

- int leadDimB

  The leading dimension of matrix B (always=1 here since numRHS always=1).

- Real rcond

  Flag to use machine precision to rank singular values of A.

- int rank

  The effective rank of matrix A.

- int lwork

  The length of the work vector.

- int info

  Output flag from DGELSS subroutine.

- Real * matrixTerms

  Matrix of quadratic polynomial terms unrolled into a vector.

- Real * responseValues

  Vector of response values that correspond to the samples in matrix A.

- Real * quadCoeffs

  Vector of quadratic polynomial coefficients.

- Real * matrixS

  Temporary storage for interface to Fortran77 LAPACK subroutines.

- Real * matrixW

  Temporary storage for interface to Fortran77 LAPACK subroutines.

6.71.1 Detailed Description

Derived approximation class for quadratic polynomial regression.

The RespSurf class assumes a quadratic polynomial fit to data which has (n+1)*(n+2)/2 coefficients for n variables. A least squares estimation of the quadratic polynomial coefficients is performed using LAPACK'S linear least squares subroutine DGELSS which uses a singular value decomposition method.

The documentation for this class was generated from the following files:

- RespSurf.H
- RespSurf.C

6.72 SGOPTApplication Class Reference

Maps the evaluation functions used by SGOPT algorithms to the DAKOTA evaluation functions.

`#include <SGOPTApplication.H>`

Public Methods

- SGOPTApplication (DakotaModel &model, DakotaResponse(*multiobj_mod_ptr)(const DakotaResponse &), int type)
  constructor.
- ~SGOPTApplication ()
  destructor.
- int DoEval (OptPoint &pt, OptResponse *response, int synch_flag)
  launch a function evaluation either synchronously or asynchronously.
- int synchronize ()
  blocking retrieval of all pending jobs.
- int next_eval (int &id)
  nonblocking query and retrieval of a job if completed.
- void dakota_asynch_flag (const short &asynch_flag)
  set dakotaModelAsynchFlag.

Private Methods

- void copy (const DakotaResponse &, OptResponse &)
  copy data from a DakotaResponse object to an SGOPT OptResponse object.

Private Attributes

- DakotaModel & userDefinedModel
  reference to the SGOPTOptimizer's model passed in the constructor.
- DakotaIntArray activeSetVector
  copy/conversion of the SGOPT request vector.
- short dakotaModelAsynchFlag
  a flag for asynchronous DAKOTA evaluations.
- DakotaList< DakotaResponse > dakotaResponseList

list of DAKOTA responses returned by synchronize_nowait().

- DakotaIntList dakotaCompletionList
  list of DAKOTA completions returned by synchronize_nowait_completions().
- size_t numObjFns
  number of objective functions.
- size_t numNonlinCons
  number of nonlinear constraints.
- DakotaResponse(* multiobjModifyPtr)(const DakotaResponse &)
  function pointer to DakotaOptimizer::multi_objective_modify() for reducing multiple objective functions to a single function.

6.72.1 Detailed Description

Maps the evaluation functions used by SGOPT algorithms to the DAKOTA evaluation functions.

SGOPTApplication is a DAKOTA class that is derived from SGOPT's AppInterface hierarchy. It redefines a variety of virtual SGOPT 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.

6.72.2 Member Function Documentation

6.72.2.1 int SGOPTApplication::DoEval (OptPoint & *pt*, OptResponse * *prob_response*, int *synch_flag*)

launch a function evaluation either synchronously or asynchronously.

Converts SGOPT variables and request vector to DAKOTA variables and active set vector, performs a DAKOTA function evaluation with synchronization governed by synch_flag, and then copies the DakotaResponse data to the SGOPT response (synchronous) or bookkeeps the SGOPT response object (asynchronous).

6.72.2.2 int SGOPTApplication::synchronize ()

blocking retrieval of all pending jobs.

Blocking synchronize of asynchronous DAKOTA jobs followed by conversion of the DakotaResponse objects to SGOPT response objects.

6.72.2.3 int SGOPTApplication::next_eval (int & *id*)

nonblocking query and retrieval of a job if completed.

Nonblocking job retrieval. Finds a completion (if available), populates the SGOPT response, and sets id to the completed job's id. Else set id = -1.

6.72.2.4 void SGOPTApplication::dakota_asynch_flag (const short & *asynch_flag*) [inline]

set dakotaModelAsynchFlag.

This function is needed to publish the iterator's asynchFlag at run time (asynchFlag not available at construction).

The documentation for this class was generated from the following files:

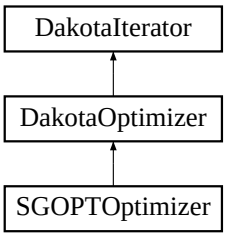
- SGOPTApplication.H
- SGOPTApplication.C

6.73 SGOPTOptimizer Class Reference

Wrapper class for the SGOPT optimization library.

`#include <SGOPTOptimizer.H>`

Inheritance diagram for SGOPTOptimizer::



Public Methods

- SGOPTOptimizer (DakotaModel &model)
  constructor.
- ~SGOPTOptimizer ()
  destructor.
- void find_optimum ()
  Performs the iterations to determine the optimal solution.

Private Methods

- void set_method_options ()
  sets options for the methods based on user specifications.

Private Attributes

- DakotaString exploratoryMoves
  user input for desired pattern search algorithm variant.
- short discreteAppFlag
  convenience flag for integer vs. real applications.
- PM_LCG * linConGenerator
  Pointer to random number generator.
- BaseOptimizer * baseOptimizer

Pointer to SGOPT base optimizer object.

- AppInterface * sgoptApplication
  pointer to the SGOPTApplication object.
- RealOptProblem * realProblem
  pointer to RealOptProblem object.
- IntOptProblem * intProblem
  pointer to IntOptProblem object.
- PGAreal * pGARealOptimizer
  pointer to PGAreal object.
- PGAint * pGAIntOptimizer
  pointer to PGAint object.
- EPSA * ePSAOptimizer
  pointer to EPSA object.
- PatternSearch * patternSearchOptimizer
  pointer to PatternSearch object.
- APPSOpt * aPPSOptimizer
  pointer to APPSOpt object.
- SWOpt * sWOptimizer
  pointer to SWOpt object.
- sMCreal * sMCrealOptimizer
  pointer to sMCreal object.

6.73.1 Detailed Description

Wrapper class for the SGOPT optimization library.

The SGOPTOptimizer class provides a wrapper for SGOPT, a Sandia-developed C++ optimization library of genetic algorithms, pattern search methods, and other nongradient-based techniques. It uses an SGOPTApplication object to perform the function evaluations.

The user input mappings are as follows: `max_iterations`, `max_function_evaluations`, `convergence_tolerance`, `solution_accuracy` and `max_cpu_time` are mapped into SGOPT's `max_iters`, `max_neval`, `ftol`, `accuracy`, and `max_time` data attributes. An `output` setting of `verbose` is passed to SGOPT's set_output() function and a setting of `debug` activates output of method initialization and sets the SGOPT `debug` attribute to 10000. SGOPT methods assume asynchronous operations whenever the algorithm has independent evaluations which can be performed simultaneously (implicit parallelism). Therefore, parallel configuration is not mapped into the method, rather it is used in SGOPTApplication to control whether or not an asynchronous evaluation request from the method is honored by the model (exception: pattern search exploratory moves is set to `best_all` for parallel function evaluations). Refer to [Hart, W.E., 1997] for additional information on SGOPT objects and controls.

6.73.2 Constructor & Destructor Documentation

6.73.2.1 SGOPTOptimizer::SGOPTOptimizer (DakotaModel & *model*)

constructor.

The constructor allocates the objects and populates the class member pointer attributes.

6.73.2.2 SGOPTOptimizer::~SGOPTOptimizer ()

destructor.

The destructor deallocates the class member pointer attributes.

6.73.3 Member Function Documentation

6.73.3.1 void SGOPTOptimizer::find_optimum () [virtual]

Performs the iterations to determine the optimal solution.

find_optimum redefines the DakotaOptimizer virtual function to perform the optimization using SGOPT. It first sets up the problem data, then executes minimize() on the SGOPT algorithm, and finally catalogues the results.

Reimplemented from DakotaOptimizer.

6.73.3.2 void SGOPTOptimizer::set_method_options () [private]

sets options for the methods based on user specifications.

set_method_options propagates DAKOTA user input to the appropriate SGOPT objects.

6.73.4 Member Data Documentation

6.73.4.1 AppInterface* SGOPTOptimizer::sgoptApplication [private]

pointer to the SGOPTApplication object.

SGOPTApplication is a DAKOTA class derived from the SGOPT AppInterface class. It redefines the virtual SGOPT evaluation functions to use DAKOTA evaluation functions.

The documentation for this class was generated from the following files:

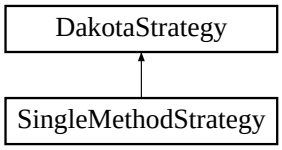
- SGOPTOptimizer.H
- SGOPTOptimizer.C

6.74 SingleMethodStrategy Class Reference

Simple fall-through strategy for running a single iterator on a single model.

`#include <SingleMethodStrategy.H>`

Inheritance diagram for SingleMethodStrategy::



Public Methods

- SingleMethodStrategy (ProblemDescDB &problem_db)
  constructor.
- ~SingleMethodStrategy ()
  destructor.
- void run_strategy ()
  Perform the strategy by executing selectedIterator on userDefinedModel.

Private Attributes

- DakotaModel userDefinedModel
  the model to be iterated.
- DakotaIterator selectedIterator
  the iterator.

6.74.1 Detailed Description

Simple fall-through strategy for running a single iterator on a single model.

This strategy executes a single iterator on a single model. Since it does not provide coordination for multiple iterators and models, it can considered to be a ”fall-through” strategy in that it allows control to fall through immediately to the iterator.

The documentation for this class was generated from the following files:

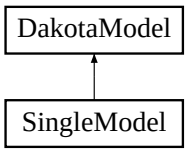
- SingleMethodStrategy.H
- SingleMethodStrategy.C

6.75 SingleModel Class Reference

Derived model class which utilizes a single interface to map variables into responses.

`#include <SingleModel.H>`

Inheritance diagram for SingleModel::



Public Methods

- SingleModel (ProblemDescDB &problem_db)

  constructor.

- ~SingleModel ()

  destructor.

- void derived_compute_response (const DakotaIntArray &asv)

  portion of compute_response() specific to SingleModel (invokes a synchronous map() on userDefinedInterface).

- void derived_asynch_compute_response (const DakotaIntArray &asv)

  portion of asynch_compute_response() specific to SingleModel (invokes an asynchronous map() on userDefinedInterface).

- const DakotaArray< DakotaResponse > & derived_synchronize ()

  portion of synchronize() specific to SingleModel (invokes synch() on userDefinedInterface).

- const DakotaList< DakotaResponse > & derived_synchronize_nowait ()

  portion of synchronize_nowait() specific to SingleModel (invokes synch_nowait() on userDefinedInterface).

- DakotaString local_eval_synchronization ()

  return userDefinedInterface synchronization setting.

- const DakotaIntList & synchronize_nowait_completions ()

  return completion id's matching response list from synchronize_nowait (request forwarded to userDefinedInterface).

- short derived_master_overload () const

  flag which prevents overloading the master with a multiprocessor evaluation (request forwarded to userDefinedInterface).

- void derived_init_communicators (const DakotaIntArray &message_lengths, const int &max_iterator_concurrency)

  portion of init_communicators() specific to SingleModel (request forwarded to userDefinedInterface).

- void free_communicators ()

  deallocate communicator partitions for the SingleModel (request forwarded to userDefinedInterface).

- void serve ()

  Service job requests received from the master. Completes when a termination message is received from stop_servers() (request forwarded to userDefinedInterface).

- void stop_servers ()

  executed by the master to terminate all slave server operations on a particular model when iteration on that model is complete (request forwarded to userDefinedInterface).

- int total_eval_counter () const

  return the total evaluation count for the SingleModel (request forwarded to userDefinedInterface).

- int new_eval_counter () const

  return the new evaluation count for the SingleModel (request forwarded to userDefinedInterface).

Private Attributes

- DakotaInterface userDefinedInterface

  the interface used for mapping variables to responses.

6.75.1 Detailed Description

Derived model class which utilizes a single interface to map variables into responses.

The SingleModel class is the simplest of the derived model classes. It provides the capabilities the old DakotaModel class, prior to the development of layered and nested model extensions. The derived response computation and synchronization functions utilize a single interface to perform the function evaluations.

The documentation for this class was generated from the following files:

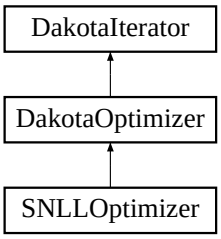
- SingleModel.H
- SingleModel.C

6.76 SNLLOptimizer Class Reference

Wrapper class for the OPT++ optimization library.

`#include <SNLLOptimizer.H>`

Inheritance diagram for SNLLOptimizer::



Public Methods

- SNLLOptimizer (DakotaModel &model)

  constructor.

- ~SNLLOptimizer ()

  destructor.

- void find_optimum ()

  Performs the iterations to determine the optimal solution.

Static Private Methods

- void init_fn (int n, ColumnVector &x)

  An initialization mechanism provided by OPT++ (not currently used).

- void nlf0_evaluator (int n, const ColumnVector &x, Real &f, int &result_mode)

  objective function evaluator function for OPT++ methods which require only function values.

- void fdnlf1_evaluator (int n, const ColumnVector &x, Real &f, int &result_mode)

  objective function evaluator function which provides function values to OPT++ methods for computing numerical gradients by finite differences.

- void nlf1_evaluator (int mode, int n, const ColumnVector &x, Real &f, ColumnVector &g, int &result_mode)

  objective function evaluator function which provides function values and gradients to OPT++ methods.

- void nlf2_evaluator (int mode, int n, const ColumnVector &x, Real &f, ColumnVector &g, SymmetricMatrix &h, int &result_mode)

objective function evaluator function which provides function values, gradients, and Hessians to OPT++ methods.

- void nlf2_evaluator_gn (int mode, int n, const ColumnVector &x, Real &fx, ColumnVector &grad, SymmetricMatrix &hess, 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.

- void constraint0_evaluator (int n, const ColumnVector &x, ColumnVector &f, int &result_mode)

  constraint evaluator function for OPT++ methods which require only constraint values.

- void constraint1_evaluator (int mode, int n, const ColumnVector &x, ColumnVector &f, Matrix &g, int &result_mode)

  constraint evaluator function which provides constraint values and gradients to OPT++ methods.

- void constraint2_evaluator (int mode, int n, const ColumnVector &x, ColumnVector &f, Matrix &g, OptppArray< SymmetricMatrix > &h, int &result_mode)

  constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ methods.

Private Attributes

- DakotaString searchMethod

  value_based_line_search, gradient_based_line_search, trust_region, or tr_pds.

- SearchStrategy s

  enum: LineSearch, TrustRegion, or TrustPDS.

- MeritFcn mfcn

  enum: NormFmu, ArgaezTapia, or VanShanno.

- short vendorNumericalGradFlag

  flags numerical gradients via the internal OPT++ finite differencing routine.

- NLP0 * nlfObjective

  objective NLF base class pointer.

- NLP0 * nlfConstraint

  constraint NLF base class pointer.

- NLP * nlpConstraint

  constraint NLP pointer.

- NLF0 * nlf0

  pointer to objective NLF for nongradient optimizers.

- NLF1 * nlf1

  pointer to objective NLF for (analytic) gradient optimizers.

- NLF1 * nlf1Con

  pointer to constraint NLF for (analytic) gradient optimizers.

- FDNLF1 * fdnlf1

  pointer to objective NLF for (finite diff) gradient optimizers.

- FDNLF1 * fdnlf1Con

  pointer to constraint NLF for (finite diff) gradient optimizers.

- NLF2 * nlf2

  pointer to objective NLF for full Newton optimizers.

- NLF2 * nlf2Con

  pointer to constraint NLF for full Newton optimizers.

- NLF1 * bcnlf1

  pointer to objective NLF for bound constrained (analytic) gradient optimizers.

- FDNLF1 * bcfdnlf1

  pointer to objective NLF for bound constrained (finite diff) gradient optimizers.

- NLF2 * bcnlf2

  pointer to objective NLF for bound constrained full Newton optimizers.

- OptimizeClass * theOptimizer

  optimizer base class pointer.

- OptPDS * optpds

  PDS optimizer pointer.

- OptCG * optcg

  CG optimizer pointer.

- OptNewton * optnewton

  Newton optimizer pointer.

- OptQNewton * optqnewton

  Quasi-Newton optimizer pointer.

- OptFDNewton * optfdnewton

  Finite Difference Newton optimizer pointer.

- OptBCNewton * optbcnewton

  Bound constrained Newton optimizer pointer.

- OptBCQNewton * optbcqnewton

  Bound constr Quasi-Newton optimizer pointer.

- OptBaNewton * optbanewton

  Barrier Newton optimizer pointer.

- OptBaQNewton * optbaqnewton

  Barrier Quasi-Newton optimizer pointer.

- OptBCEllipsoid * optbcellipsoid

  Bound constrained ellipsoid pointer.

- OptNIPS * optnips

  NIPS optimizer pointer.

- OptQNIPS * optqnips

  Quasi-Newton NIPS optimizer pointer.

- OptFDNIPS * optfdnips

  Finite Difference NIPS optimizer pointer.

Static Private Attributes

- int staticSpeculativeFlag

  flags speculative gradient logic (for parallel load-balancing).

- int staticModeOverrideFlag

  flags OPT++ mode override (for combining value, gradient, and Hessian requests).

- DakotaRealVector staticConstraintValues

  vector of nonlinear constraints.

- int staticNumNonlinearEqConstraints

  number of nonlinear equality constraints.

- int staticNumNonlinearIneqConstraints

  number of nonlinear inequality constraints.

6.76.1 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 or static as well. To isolate the effect of these static requirements from the rest of the iterator hierarchy, static copies are made of many non-static attributes inherited from above.

The user input mappings are as follows: `max_iterations`, `max_function_evaluations`, `convergence_tolerance`, `max_step`, `gradient_tolerance`, `search_method`, `initial_radius`, and `search_scheme_size` are set using OPT++'s setMaxIter(), setMaxFeval(), setFcnTol(),

setMaxStep(), setGradTol(), setSearchStrategy(), setInitialEllipsoid(), 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/VendorOptimizers/opt++ directory for information on OPT++ class member functions.

6.76.2 Member Function Documentation

6.76.2.1 void SNLLOptimizer::nlf0_evaluator (int *n*, const ColumnVector & *x*, Real & *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 no gradients are available. There is currently no difference between this function & fdnlf1_evaluator.

6.76.2.2 void SNLLOptimizer::fdnlf1_evaluator (int *n*, const ColumnVector & *x*, Real & *f*, int & *result_mode*) [static, private]

objective function evaluator function which provides function values to OPT++ methods for computing numerical gradients by finite differences.

For use when DAKOTA computes f and opt++'s internal finite difference capability computes df/dX. In effect, fdnlf1 is like an nlf0.

6.76.2.3 void SNLLOptimizer::nlf1_evaluator (int *mode*, int *n*, const ColumnVector & *x*, Real & *f*, ColumnVector & *g*, 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 gradientType). Vendor numerical gradient case is handled within fdnlf1_evaluator.

6.76.2.4 void SNLLOptimizer::nlf2_evaluator (int *mode*, int *n*, const ColumnVector & *x*, Real & *f*, ColumnVector & *g*, SymmetricMatrix & *h*, 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.

6.76.2.5 void SNLLOptimizer::nlf2_evaluator_gn (int *mode*, int *n*, const ColumnVector & *x*, Real & *fx*, ColumnVector & *grad*, SymmetricMatrix & *hess*, 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 DakotaResponse is made up of residual functions and their gradients with numFunctions = numLeastSquaresTerms. 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 DakotaResponse object).

The documentation for this class was generated from the following files:

- SNLLOptimizer.H
- SNLLOptimizer.C

6.77 SortCompare Class Template Reference

`#include <DakotaList.H>`

Public Methods

- SortCompare (int(∗func)(const T &, const T &))
  Constructor that defines the pointer to function.
- bool operator() (const T &p1, const T &p2) const
  The operator() must be defined. Calls the defined sortFunction.

Private Attributes

- int(∗ sortFunction)(const T &, const T &)
  Pointer to test function.

6.77.1 Detailed Description

template<class T> class SortCompare< T >

Internal Functor used in the sort algorithm to sort using a specified compare method. The class holds a pointer to the sort function.

The documentation for this class was generated from the following file:

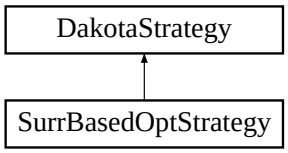
- DakotaList.H

6.78 SurrBasedOptStrategy Class Reference

Strategy for provably-convergent surrogate-based optimization.

`#include <SurrBasedOptStrategy.H>`

Inheritance diagram for SurrBasedOptStrategy::



Public Methods

- SurrBasedOptStrategy (ProblemDescDB &problem_db)

  constructor.

- ~SurrBasedOptStrategy ()

  destructor.

- void run_strategy ()

  Performs the surrogate-based optimization strategy by optimizing local, global, or hierarchical surrogates over a series of trust regions.

Private Methods

- Real compute_penalty_function (const DakotaRealVector &fn_vals)

  compute a penalty function from a set of function values.

- int hard_convergence_check (const DakotaResponse &response_center_truth)

  check for hard convergence (satisfaction of gradient FCD condition).

- int soft_convergence_check (const DakotaRealVector &c_vars_center, const DakotaRealVector &c_vars_star, const DakotaResponse &response_center_truth, const DakotaResponse &response_center_approx, const DakotaResponse &response_star_truth, const DakotaResponse &response_star_approx)

  check for soft convergence (diminishing returns).

Private Attributes

- DakotaModel approximateModel

  the surrogate model (a LayeredModel object).

- DakotaIterator selectedIterator

  the optimizer used on approximateModel.

- Real trustRegionSize

  size of the current trust region (dimensional +/- offset around center for each variable defines a hypercube).

- Real minTrustRegionSize

  a soft convergence control: stop SBO when the trust region size is reduced below the minTrustRegionSize.

- Real convergenceTol

  the optimizer convergence tolerance; used in several SBO hard and soft convergence checks.

- Real constraintTol

  a tolerance specifying the distance from a constraint boundary that is allowed before an active constraint is considered to be a violated constraint (only violated constraints are used in penalty function computations).

- Real penaltyParameter

  the penalization factor for violated constraints used in penalty function calculations; increases exponentially with iteration count.

- Real gammaContract

  trust region contraction factor.

- Real gammaExpand

  trust region expansion factor.

- Real gammaNoChange

  factor for maintaining the current trust region size (normally 1.0).

- Real fcdGradientTerm

  gradient-related term from the fraction of Cauchy decrease (FCD) calculation.

- int iterMax

  maximum number of SBO iterations.

- int convergenceFlag

  code indicating satisfaction of hard or soft convergence conditions.

- int numFns

  number of response functions.

- int numVars

  number of active continuous variables.

- int softConvCount

  number of consecutive candidate point rejections. If the count reaches softConvLimit, stop SBO.

- int softConvLimit

  the limit on consecutive candidate point rejections. If exceeded by softConvCount, stop SBO.

- short gradientFlag

  flags the use of gradients throughout the SBO process.

- short correctionFlag

  flags the use of surrogate correction techniques at the center of each trust region.

- short globalApproxFlag

  flags the use of a global data fit surrogate (rsm, ann, mars, kriging).

- short localApproxFlag

  flags the use of a local data fit surrogate (Taylor series).

- short hierarchApproxFlag

  flags the use of a hierarchical surrogate.

- short newCenterFlag

  flags the acceptance of a candidate point and the existence of a new trust region center.

- short daceCenterPtFlag

  flags the availability of the center point in the DACE evaluations for global approximations (CCD, Box-Behnken).

- size_t numObjFns

  number of objective functions.

- size_t numNonlinIneqConstr

  number of nonlinear inequality constraints.

- size_t numNonlinEqConstr

  number of nonlinear equality constraints.

- DakotaRealVector multiObjWts

  vector of multiobjective weights.

- DakotaRealVector nonlinIneqLowerBnds

  vector of nonlinear inequality constraint lower bounds.

- DakotaRealVector nonlinIneqUpperBnds

  vector of nonlinear inequality constraint upper bounds.

- DakotaRealVector nonlinEqTargets

  vector of nonlinear equality constraint targets.

6.78.1 Detailed Description

Strategy for provably-convergent surrogate-based optimization.

This strategy uses a LayeredModel to perform optimization 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.

6.78.2 Member Function Documentation

6.78.2.1 void SurrBasedOptStrategy::run_strategy () [virtual]

Performs the surrogate-based optimization strategy by optimizing 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 optimizer operates on approximations in lieu of the more expensive simulation-based response functions. The size of the trust region is varied according to the goodness of the agreement between the approximations and the true response functions.

Reimplemented from DakotaStrategy.

6.78.2.2 Real SurrBasedOptStrategy::compute_penalty_function (const DakotaRealVector & *fn_vals*) [private]

compute a penalty function from a set of function values.

The penalty function computation applies a penalty multiplier to any constraint violations and adds this to the objective function. This implementation supports multiple objectives, equality constraints, and 2-sided inequalities. A negative constraintTol can be used to provide a push-back into the feasible region.

6.78.2.3 int SurrBasedOptStrategy::hard_convergence_check (const DakotaResponse & *response_center_truth*) [private]

check for hard convergence (satisfaction of gradient FCD condition).

The hard convergence check computes a fraction of Cauchy decrease (FCD) condition using gradients. It is based on equations from Alexandrov (Structural Opt 1998). Basically, if the gradient of the penalty function at the trust region center is near zero, stop the SBO iterations. Some computed terms from this function are reused in soft_convergence_check().

6.78.2.4 int SurrBasedOptStrategy::soft_convergence_check (const DakotaRealVector & *c_vars_center*, const DakotaRealVector & *c_vars_star*, const DakotaResponse & *response_center_truth*, const DakotaResponse & *response_center_approx*, const DakotaResponse & *response_star_truth*, const DakotaResponse & *response_star_approx*) [private]

check for soft convergence (diminishing returns).

Compute soft convergence metrics (quasi-FCD, trust region ratio, number of consecutive failures, min trust region size, etc.) and use them to assess whether the convergence rate has decreased to a point where the process should be terminated (diminishing returns). Some gradient-related terms are computed in hard_convergence_check().

The documentation for this class was generated from the following files:

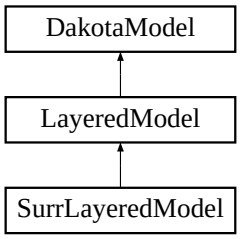
- SurrBasedOptStrategy.H
- SurrBasedOptStrategy.C

6.79 SurrLayeredModel Class Reference

Derived model class within the layered model branch for managing data fit surrogates (global and local).

`#include <SurrLayeredModel.H>`

Inheritance diagram for SurrLayeredModel::



Public Methods

- SurrLayeredModel (ProblemDescDB &problem_db)
  constructor.
- ~SurrLayeredModel ()
  destructor.

Protected Methods

- void derived_compute_response (const DakotaIntArray &asv)
  portion of compute_response() specific to SurrLayeredModel.
- void derived_asynch_compute_response (const DakotaIntArray &asv)
  portion of asynch_compute_response() specific to SurrLayeredModel.
- const DakotaArray< DakotaResponse > & derived_synchronize ()
  portion of synchronize() specific to SurrLayeredModel.
- const DakotaList< DakotaResponse > & derived_synchronize_nowait ()
  portion of synchronize_nowait() specific to SurrLayeredModel.
- short derived_master_overload () const
  flag which prevents overloading the master with a multiprocessor evaluation.
- DakotaModel & subordinate_model ()
  returns actualModel to SurrBasedOptStrategy.
- DakotaIterator & subordinate_iterator ()

return daceIterator to SurrBasedOptStrategy.

- int maximum_concurrency () const

  return the maximum concurrency available for actualModel computations during global approximation builds.

- void build_approximation ()

  Builds the local/multipoint/global approximation using daceIterator/actualModel.

- const DakotaIntList & synchronize_nowait_completions ()

  return completion id's matching response list from synchronize_nowait (request forwarded to approxInterface).

- void update_approximation (const DakotaRealVector &x_star, const DakotaResponse &response_star)

  Adds a point to a global approximation (request forwarded to approxInterface).

- int total_eval_counter () const

  return the total evaluation count for the SurrLayeredModel (request forwarded to approxInterface).

- int new_eval_counter () const

  return the new evaluation count for the SurrLayeredModel (request forwarded to approxInterface).

- void derived_init_communicators (const DakotaIntArray &message_lengths, const int &max_iterator_concurrency)

  portion of init_communicators() specific to SurrLayeredModel.

- void free_communicators ()

  deallocate communicator partitions for the SurrLayeredModel (request forwarded to actualModel).

- void serve ()

  Service job requests received from the master. Completes when a termination message is received from stop_servers() (request forwarded to actualModel).

- void stop_servers ()

  Executed by the master to terminate all slave server operations on a particular model when iteration on that model is complete (request forwarded to actualModel).

Private Attributes

- DakotaInterface approxInterface

  manages the building and subsequent evaluation of the approximations (required for both global and local).

- DakotaString actualInterfacePointer

  pointer to the actual interface from the local approximation specification (required for local); used to build actualModel for local approximations.

- DakotaString daceMethodPointer

  pointer to the dace method from the global approximation specification; used in building daceIterator and actualModel for global approximations (optional for global since restart data may also be used).

- DakotaModel actualModel

  the truth model which provides evaluations for building the surrogate (optional for global since restart data may also be used, required for local).

- DakotaIterator 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).

6.79.1 Detailed Description

Derived model class within the layered model branch for managing data fit surrogates (global and local).

The SurrLayeredModel 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.

6.79.2 Member Function Documentation

6.79.2.1 void SurrLayeredModel::derived_compute_response (const DakotaIntArray & *asv*) [inline, protected, virtual]

portion of compute_response() specific to SurrLayeredModel.

Build the approximation (if needed), evaluate the approximate response using approxInterface, and, if correction is active, correct the results.

Reimplemented from DakotaModel.

6.79.2.2 void SurrLayeredModel::derived_asynch_compute_response (const DakotaIntArray & *asv*) [inline, protected, virtual]

portion of asynch_compute_response() specific to SurrLayeredModel.

Build the approximation (if needed) and evaluate the approximate response using approxInterface in a quasi-asynchronous approach (ApproximationInterface::map() performs the map synchronously and book-keeps the results for return in derived_synchronize() below).

Reimplemented from DakotaModel.

6.79.2.3 const DakotaArray< DakotaResponse > & SurrLayeredModel::derived_synchronize () [inline, protected, virtual]

portion of synchronize() specific to SurrLayeredModel.

Retrieve quasi-asynchronous evaluations from approxInterface and, if correction is active, apply correction to each response in the array.

Reimplemented from DakotaModel.

6.79.2.4 const DakotaList< DakotaResponse > & SurrLayeredModel::derived_synchronize_nowait () [inline, protected, virtual]

portion of synchronize_nowait() specific to SurrLayeredModel.

Retrieve quasi-asynchronous evaluations from approxInterface and, if correction is active, apply correction to each response in the list.

Reimplemented from DakotaModel.

6.79.2.5 short SurrLayeredModel::derived_master_overload () const [inline, protected, virtual]

flag which prevents overloading the master with a multiprocessor evaluation.

compute_response calls never overload the master since there is no parallelism in the use of approxInterface.

Reimplemented from DakotaModel.

6.79.2.6 int SurrLayeredModel::maximum_concurrency () const [protected, virtual]

return the maximum concurrency available for actualModel computations during global approximation builds.

Return the greater of the dace samples user-specification or the min_samples approximation requirement. min_samples does not have to account for reuse_samples, since this will vary (assume 0).

Reimplemented from DakotaModel.

6.79.2.7 void SurrLayeredModel::build_approximation () [protected, virtual]

Builds the local/multipoint/global approximation using daceIterator/actualModel.

Build either a global approximation using daceIterator or a local approximation using actualModel. Selection triggers on actualInterfacePointer (required specification for local approximation interfaces, not used in global specification).

Reimplemented from DakotaModel.

6.79.2.8 void SurrLayeredModel::derived_init_communicators (const DakotaIntArray & *message_lengths*, const int & *max_iterator_concurrency*) [inline, protected, virtual]

portion of init_communicators() specific to SurrLayeredModel.

asynchronous flags need to be initialized for the sub-models. In addition, max_iterator_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 DakotaModel.

6.79.3 Member Data Documentation

6.79.3.1 DakotaString SurrLayeredModel::actualInterfacePointer [private]

pointer to the actual interface from the local approximation specification (required for local); used to build actualModel for local approximations.

Specification is used only for local approximations, since the dace_method_pointer in the global approximation specification is responsible for identifying all actualModel components.

6.79.3.2 DakotaModel SurrLayeredModel::actualModel [private]

the truth model which provides evaluations for building the surrogate (optional for global since restart data may also be used, required for local).

There are no restrictions on actualModel in the global case, so arbitrary nestings are possible. In the local case, model_type must be set to "single" to avoid recursion on SurrLayeredModel, since there is no additional method specification.

The documentation for this class was generated from the following files:

- SurrLayeredModel.H
- SurrLayeredModel.C

6.80 SurrogateDataPoint Class Reference

Simple container class encapsulating basic parameter and response data for defining a ”truth” data point.

`#include <DakotaApproximation.H>`

Public Methods

- SurrogateDataPoint ()
  default constructor.
- SurrogateDataPoint (const DakotaRealVector &x, const Real &f, const DakotaRealVector &grad_f)
  standard constructor.
- SurrogateDataPoint (const SurrogateDataPoint &sdp)
  copy constructor.
- ~SurrogateDataPoint ()
  destructor.
- int operator== (const SurrogateDataPoint &sdp) const
  equality operator.
- SurrogateDataPoint & operator= (const SurrogateDataPoint &sdp)
  assignment operator.

Public Attributes

- DakotaRealVector continuousVars
  continuous variables.
- Real responseFn
  truth response function value.
- DakotaRealVector responseGrad
  truth response function gradient.

6.80.1 Detailed Description

Simple container class encapsulating basic parameter and response data for defining a ”truth” data point.

A list of these data points is contained in each DakotaApproximation instance (DakotaApproximation::currentPoints) and provides the data to build the approximation. Data is public to avoid maintaining set/get functions, but is still encapsulated within DakotaApproximation since

DakotaApproximation::currentPoints is protected (a similar model is used with with Data class objects contained in ProblemDescDB and with ParallelismLevel objects contained in ParallelLibrary).

The documentation for this class was generated from the following file:

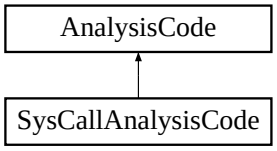
- DakotaApproximation.H

6.81 SysCallAnalysisCode Class Reference

Derived class in the AnalysisCode class hierarchy which spawns simulations using system calls.

`#include <SysCallAnalysisCode.H>`

Inheritance diagram for SysCallAnalysisCode::



Public Methods

- SysCallAnalysisCode (const ProblemDescDB &problem_db)

  constructor.

- ~SysCallAnalysisCode ()

  destructor.

- void spawn_evaluation (const short block_flag)

  spawn a complete function evaluation.

- void spawn_input_filter (const short block_flag)

  spawn the input filter portion of a function evaluation.

- void spawn_analysis (const int &analysis_id, const short block_flag)

  spawn a single analysis as part of a function evaluation.

- void spawn_output_filter (const short block_flag)

  spawn the output filter portion of a function evaluation.

- const DakotaString & command_usage () const

  return commandUsage.

Private Attributes

- DakotaString commandUsage

  optional command usage string for supporting nonstandard command syntax (supported only by SysCall analysis codes).

6.81.1 Detailed Description

Derived class in the AnalysisCode class hierarchy which spawns simulations using system calls.

SysCallAnalysisCode creates separate simulation processes using the C system() command. It utilizes CommandShell to manage shell syntax and asynchronous invocations.

6.81.2 Member Function Documentation

6.81.2.1 void SysCallAnalysisCode::spawn_evaluation (const short *block_flag*)

spawn a complete function evaluation.

Put the SysCallAnalysisCode to the shell using either the default syntax or specified commandUsage syntax. This function is used when all portions of the function evaluation (i.e., all analysis drivers) are executed on the local processor.

6.81.2.2 void SysCallAnalysisCode::spawn_input_filter (const short *block_flag*)

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.

6.81.2.3 void SysCallAnalysisCode::spawn_analysis (const int & *analysis_id*, const short *block_flag*)

spawn a single analysis as part of a function evaluation.

Put a single analysis to the shell using the default syntax (no commandUsage support for analyses). 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.

6.81.2.4 void SysCallAnalysisCode::spawn_output_filter (const short *block_flag*)

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.

The documentation for this class was generated from the following files:

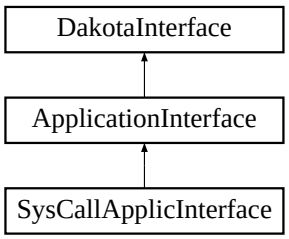
- SysCallAnalysisCode.H
- SysCallAnalysisCode.C

6.82 SysCallApplicInterface Class Reference

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

`#include <SysCallApplicInterface.H>`

Inheritance diagram for SysCallApplicInterface::



Public Methods

- SysCallApplicInterface (const ProblemDescDB &problem_db, const size_t &num_fns)

  constructor.

- ~SysCallApplicInterface ()

  destructor.

- void derived_map (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &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 derived_synch (DakotaList< ParamResponsePair > &prp_list)

  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 derived_synch_nowait (DakotaList< ParamResponsePair > &prp_list)

  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 derived_synchronous_local_analysis (const 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().

Private Methods

- void spawn_application (const short block_flag)

  Spawn the application by managing the input filter, analysis drivers, and output filter. Called from derived_map() & derived_map_asynch().

- void derived_synch_kernel (DakotaList< ParamResponsePair > &prp_list)

  Convenience function for common code between derived_synch() & derived_synch_nowait().

- short system_call_file_test (const DakotaString &root_file)

  detect completion of a function evaluation through existence of the necessary results file(s).

Private Attributes

- SysCallAnalysisCode sysCallSimulator

  SysCallAnalysisCode provides convenience functions for passing the input filter, the analysis drivers, and the output filter to a CommandShell in various combinations.

- DakotaIntList sysCallList

  list of function evaluation id's for active asynchronous system call evaluations.

- DakotaIntList failIdList

  list of function evaluation id's for tracking response file read failures.

- DakotaIntList failCountList

  list containing the number of response read failures for each function evaluation identified in failIdList.

6.82.1 Detailed Description

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

SysCallApplicInterface uses a SysCallAnalysisCode object for performing simulation invocations.

The documentation for this class was generated from the following files:

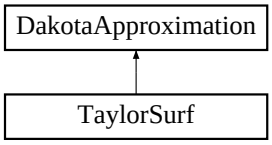
- SysCallApplicInterface.H
- SysCallApplicInterface.C

6.83 TaylorSurf Class Reference

Derived approximation class for 1st order Taylor series (local approximation).

`#include <TaylorSurf.H>`

Inheritance diagram for TaylorSurf::



Public Methods

- TaylorSurf (const ProblemDescDB &problem_db)

  constructor.

- ~TaylorSurf ()

  destructor.

Protected Methods

- void find_coefficients ()

  calculate the data fit coefficients using the currentPoints list of SurrogateDataPoints.

- int required_samples (int num_vars)

  return the minimum number of samples required to build the derived class approximation type in num_vars dimensions.

- Real get_value (const DakotaRealVector &x)

  retrieve the approximate function value for a given parameter vector.

- const DakotaRealVector & get_gradient (const DakotaRealVector &x)

  retrieve the approximate function gradient for a given parameter vector.

6.83.1 Detailed Description

Derived approximation class for 1st order Taylor series (local approximation).

The TaylorSurf class provides a local approximation based on data from a single point in parameter space. It uses a first order Taylor series expansion: f(x) = f(x_c) + grad(x_c) * (x - x_c)

The documentation for this class was generated from the following files:

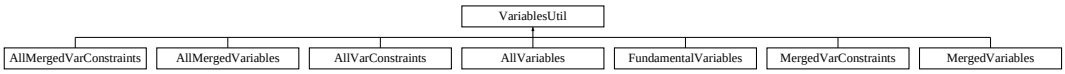
- TaylorSurf.H
- TaylorSurf.C

6.84 VariablesUtil Class Reference

Utility class for the DakotaVariables and DakotaVarConstraints hierarchies which provides convenience functions for variable vectors and label arrays for combining design, uncertain, and state variable types and merging continuous and discrete variable domains.

`#include <VariablesUtil.H>`

Inheritance diagram for VariablesUtil::



Public Methods

- VariablesUtil ()

  constructor.

- ~VariablesUtil ()

  destructor.

Protected Methods

- void update_merged (const DakotaRealVector &c_array, const DakotaIntVector &d_array, DakotaRealVector &m_array)

  combine a continuous array and a discrete array into a single continuous array through promotion of integers to reals (merged view).

- void update_all_continuous (const DakotaRealVector &c1_array, const DakotaRealVector &c2_array, const DakotaRealVector &c3_array, DakotaRealVector &all_array) const

  combine 3 continuous arrays (design, uncertain, state) into a single continuous array (all view).

- void update_all_discrete (const DakotaIntVector &d1_array, const DakotaIntVector &d2_array, DakotaIntVector &all_array) const

  combine 2 discrete arrays (design, state) into a single discrete array (all view).

- void update_labels (const DakotaStringArray &l1_array, const DakotaStringArray &l2_array, DakotaStringArray &all_array)

  combine 2 label arrays into a single label array (merged or all views).

- void update_labels (const DakotaStringArray &l1_array, const DakotaStringArray &l2_array, const DakotaStringArray &l3_array, DakotaStringArray &all_array)

  combine 3 label arrays (design, uncertain, state) into a single label array (all view).

6.84.1 Detailed Description

Utility class for the DakotaVariables and DakotaVarConstraints hierarchies which provides convenience functions for variable vectors and label arrays for combining design, uncertain, and state variable types and merging continuous and discrete variable domains.

Derived classes within the DakotaVariables and DakotaVarConstraints hierarchies use multiple inheritance to inherit these utilities.

The documentation for this class was generated from the following file:

- VariablesUtil.H

Chapter 7

DAKOTA File Documentation

7.1 keywordtable.C File Reference

file containing keywords for the strategy, method, variables, interface, and responses input specifications from **dakota.input.spec**.

Variables

- const struct KeywordHandler idrKeywordTable [ ]

  Initialize the keyword table as a vector of KeywordHandler structures (KeywordHandler declared in idr-keyword.h). A null KeywordHandler structure signifies the end of the keyword table.

7.1.1 Detailed Description

file containing keywords for the strategy, method, variables, interface, and responses input specifications from **dakota.input.spec**.

7.2 main.C File Reference

file containing the main program for DAKOTA.

Functions

- void manage_inputs (int argc, char **argv, ProblemDescDB &problem_db, CommandLineHandler &cmd_line_handler)

  manage command line inputs, parse the input file, and populate the problem description database.

- void manage_outputs (ofstream &output_ofstream, ofstream &error_ofstream, const ParallelLibrary &parallel_lib)

  manage output streams if required.

- void manage_restart (CommandLineHandler &cmd_line_handler, ParallelLibrary &parallel_lib)

  manage the restart file(s).

- void clean_up (ofstream &output_ofstream, ofstream &error_ofstream, const ParallelLibrary &parallel_lib)

  close output streams.

- int main (int argc, char *argv[ ])

  The main DAKOTA program.

Variables

- DakotaList< ParamResponsePair > data_pairs

  list of all param/response pairs.

- DakotaBoStream * write_restart

  the restart binary output stream.

- ofstream write_ostream

  Rogue Wave requirement for binary streams.

- int write_precision = 10

  used in ostream data output fns.

7.2.1 Detailed Description

file containing the main program for DAKOTA.

7.2.2 Function Documentation

7.2.2.1 void manage_inputs (int *argc*, char ** *argv*, ProblemDescDB & *problem_db*, CommandLineHandler & *cmd_line_handler*)

manage command line inputs, parse the input file, and populate the problem description database.

Manage command line inputs using the CommandLineHandler class and parse the input file using the Input Deck Reader (IDR) parsing system. IDR populates the ProblemDescDB object with the input file data.

7.2.2.2 void manage_outputs (ofstream & *output_ofstream*, ofstream & *error_ofstream*, const ParallelLibrary & *parallel_lib*)

manage output streams if required.

If concurrent iterators are to be used, create and tag multiple output streams in order to prevent jumbled output. This uses the CommonIO facility from UTILIB.

7.2.2.3 void manage_restart (CommandLineHandler & *cmd_line_handler*, ParallelLibrary & *parallel_lib*)

manage the restart file(s).

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.

7.2.2.4 void clean_up (ofstream & *output_ofstream*, ofstream & *error_ofstream*, const ParallelLibrary & *parallel_lib*)

close output streams.

Close streams associated with manage_inputs, manage_outputs, and manage_restart.

7.2.2.5 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 DakotaStrategy and invoke its run_strategy() virtual function.

7.3 restart_util.C File Reference

file containing the DAKOTA restart utility main program.

Functions

- void print_restart (int argc, char **argv, DakotaString print_dest)
  print a restart file.
- void print_restart_tabular (int argc, char **argv, DakotaString print_dest)
  print a restart file (tabular format).
- void read_neutral (int argc, char **argv)
  read a restart file (neutral file format).
- void repair_restart (int argc, char **argv)
  repair a restart file by removing corrupted evaluations.
- void concatenate_restart (int argc, char **argv)
  concatenate multiple restart files.
- int main (int argc, char *argv[ ])
  The main program for the DAKOTA restart utility.

Variables

- DakotaBoStream * write_restart
  the restart binary output stream.
- ofstream write_ostream
  Rogue Wave requirement for binary streams.
- int write_precision = 16
  used in ostream output fns. DAKOTA's main.C sets this to 10, however "print" outputs parameters in full precision (16 digits for double).

7.3.1 Detailed Description

file containing the DAKOTA restart utility main program.

7.3.2 Function Documentation

7.3.2.1 void print_restart (int *argc*, char ** *argv*, DakotaString *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.

7.3.2.2 void print_restart_tabular (int *argc*, char ** *argv*, DakotaString *print_dest*)

print a restart file (tabular format).

Usage: "dakota_restart_util to_pdb dakota.rst dakota.pdb"

"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).

7.3.2.3 void read_neutral (int *argc*, char ** *argv*)

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.

7.3.2.4 void repair_restart (int *argc*, char ** *argv*)

repair a restart file by removing corrupted evaluations.

Usage: "dakota_restart_util remove 0.0 dakota_old.rst dakota_new.rst"

Removes all evals for which one of the function values matches argv[2].

7.3.2.5 void concatenate_restart (int *argc*, char ** *argv*)

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.

7.3.2.6 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()).

Chapter 8

Recommended Practices for DAKOTA Development

8.1 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. As a result, C++ coding styles are fairly standard across a variety of Sandia software projects in the engineering and computational sciences.

8.2 Style Guidelines

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

8.2.1 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) are upper case, with underscores separating words, e.g.:

```
const double CONSTANT_VALUE;
```

8.2.2 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 arose from the desire to have member functions which set and return the value of a 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 DakotaRealVector& c_vars) { // set
  continuousVariables = c_vars;
}
const DakotaRealVector& 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.:

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

8.2.3 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” in the Options pull down menu). Other helpful features include ”Paren highlighting” for matching parentheses (Options pull down menu) and the ”New Frame” utility (File pull down menu) 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 X-window 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 DakotaString& 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).

8.3 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 be identical to the class name defined by that file. Exceptions: in some 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 (e.g., DakotaResponse.C/.H files contain DakotaResponse and DakotaResponseRep classes) or some generalization of the set of classes (e.g., DakotaBinStream.C/.H files contain the DakotaBiStream/DakotaBoStream classes for binary input and binary output).

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

- **.H** A class header file ends in the suffix .H. 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.
- **.C** A class implementation file ends in the suffix .C. 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.

8.4 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 .C 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:       DakotaModel
//- Description: The model to be iterated.  Contains DakotaVariables,
//-              DakotaInterface, and DakotaResponse objects.
//- Owner:       Mike Eldred
//- Version: $Id: RecommendPract.dox,v 1.4 2001/11/08 21:33:31 mseldre Exp $
```

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.

Chapter 9

Instructions for Modifying DAKOTA's Input Specification

9.1 Modify dakota.input.spec

The master input specification resides in **$DAKOTA/src/dakota.input.spec**. As part of the Input Deck Reader (IDR) build process, a soft link to this file is created in $DAKOTA/VendorPackages/idr. The master input specification can be modified with the addition of new constructs using the following logical relationships:

- {} for required individual specifications
- () for required group specifications
- [] for optional individual specifications
- [] for optional group specifications
- | for "or" conditionals

These constructs can be used to define a variety of dependency relationships in the input specification. It is recommended that you review the existing specification and have an understanding of the constructs in use before attempting to add new constructs.

Warning:

- Do *not* skip this step. Attempts to modify the keywordtable.C and ProblemDescDB.C files in $DAKOTA/src without reference to the results of the code generator are very error-prone. Moreover, the input specification provides a reference to the allowable inputs of a particular executable and should be kept in synch with the parser files (modifying the parser files independent of the input specification creates, at a minimum, undocumented features).
- Since the Input Deck Reader (IDR) parser allows abbreviation of keywords, you *must* avoid adding a keyword that could be misinterpreted as an abbreviation for a different keyword within the same keyword handler (the term "keyword handler" refers to the strategy_kwhandler(), method_kwhandler(), variables_kwhandler(), interface_kwhandler(), and responses_kwhandler() member functions in the ProblemDescDB class). 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 specification.

- Since IDR input is order-independent, the same keyword may be reused multiple times in the specification if and only if the specification blocks are mutually exclusive. For example, method selections (e.g., `dot_frcg`, `dot_bfgs`) can reuse the same method setting keywords (e.g., `optimization_type`) since the method selection blocks are all separated by logical "or"'s. If `dot_frcg` and `dot_bfgs` were not exclusive and could be specified at the same time, then association of the `optimization_type` setting with a particular method would be ambiguous. This is the reason why repeated specifications which are non-exclusive must be made unique, typically with a prepended identifier (e.g., `cdv_initial_point`, `ddv_initial_point`).

9.2 Rebuild IDR

```
cd $DAKOTA/VendorPackages/idr
make clean
make
```

These steps regenerate keywordtable.C and idr-gen-code.C in the $DAKOTA/VendorPackages/idr/<canonical_build_directory> directory for use in updating keywordtable.C and ProblemDescDB.C in $DAKOTA/src.

9.3 Update keywordtable.C in $DAKOTA/src

Do *not* directly replace the keywordtable.C in $DAKOTA/src using the one from idr, as there are important differences in the kwhandler bindings. Rather, update the keywordtable.C in $DAKOTA/src using the one from idr as a reference. Once this step is completed, it is a good idea to verify the match by diff'ing the 2 files. The only differences should be in comments, includes, and kwhandler declarations.

9.4 Update ProblemDescDB.C in $DAKOTA/src

Find the keyword handler functions (e.g., variables_kwhandler()) in $DAKOTA/VendorPackages/idr/<canonical_build_directory>/idr-gen-code.C and $DAKOTA/src/ProblemDescDB.C which correspond to your modifications to the input specification. The idr-gen-code.C file is the result of a code generator and contains skeleton constructs for extracting data from IDR. You will be copying over parts of this skeleton to ProblemDescDB.C and then adding code to populate attributes within Data class container objects.

9.4.1 Replace keyword handler declarations and counter loop

Rather than trying to update these line by line, it is recommended to delete the entire block starting with the keyword declarations and ending at the bottom of the keyword counter loop. The declarations assign -1 to keywords and look like this:

```
Int cdv_descriptor = -1;
Int cdv_initial_point = -1;
```

They start after the line ”Int cntr;”. The keyword counter loop looks like this:

```
for  ( cntr=data_len; cntr--; ) {
  if  ( idr_find_id( &cdv_descriptor, cntr,
                "cdv_descriptor", id_str, kw_str ) ) continue;
  ...
  if  ( idr_find_id( &wuv_dist_upper_bounds, cntr,
                "wuv_dist_upper_bounds", id_str, kw_str ) ) continue;
}
```

Once the old keyword declarations and keyword counter loop have been deleted, replace them with the corresponding blocks from idr-gen-code.C containing the updated keyword declarations and counter loop.

9.4.2 Update keyword handler logic blocks

For the newly added or modified input specifications, copy the appropriate skeleton constructs from idr-gen-code.C and paste them into the corresponding location in ProblemDescDB.C.

The next step is to add code to these skeletons to set data attributes within the Data class object used by the keyword handler. At the top of each keyword handler, a Data class object is instantiated, e.g.:

```
DataMethod data_method;
```

Each data class is a simple container class which contains the data from a single keyword handler invocation. Within each skeleton construct, you will extract data from the IDR data structures and then use this data to set the corresponding attribute within the Data class.

Integer, real, and string data are extracted using the `idata`, `rdata`, and `cdata` arrays provided by IDR. These arrays are indexed using a bracket operator with the keyword as an index.

Lists of integer and real data are extracted using the `idr_table` constructs provided by IDR. Unfortunately, IDR does not provide an `idr_table` for string data, so these extractions are more involved. Refer to existing `<LISTof><STRING>` extractions for use as a model.

Example 1: if you added the specification:

```
[method_setting = <REAL>]
```

you would copy over

```
if  ( method_setting >= 0 ) {
}
```

from idr-gen-code.C into ProblemDescDB.C and then populate the if block with a call to set the corresponding attribute within the `data_method` object using data extracted using the `rdata` array:

```
if  ( method_setting >= 0 ) {
  data_method.methodSetting = rdata[method_setting];
}
```

Use of a set member function within DataMethod is not needed since the data is public. The data is public since ProblemDescDB already provides sufficient encapsulation (ProblemDescDB::methodList, ProblemDescDB::variablesList, ProblemDescDB::interfaceList, and ProblemDescDB::responsesList are private attributes), and no other classes have direct access. A similar model is used with SurrogateDataPoint objects contained in DakotaApproximation (DakotaApproximation::currentPoints) and with ParallelismLevel objects contained in ParallelLibrary (ParallelLibrary::parallelismLevels). Allowing public access to the Data class attributes is essentially equivalent to declaring ProblemDescDB a friend, but with the important bonus of a significant reduction in the amount code to maintain. That is, the Data classes can be streamlined (and the work in modifying the input specification can be reduced) by omitting set/get functions.

Example 2: if you added the specification

```
[method_setting = <LISTof><REAL>]
```

you would copy over

```
if  ( method_setting >= 0 ) {
  { Int idr_table_len;
    Real**  idr_table = idr_get_real_table( parsed_data, method_setting,
                                            idr_table_len, 1, 1 );
  }
}
```

from idr-gen-code.C into ProblemDescDB.C and then populate it with a loop which extracts each entry of the table and populates the corresponding attribute within the `data_method` object. The `idr_table_len` attribute is used for the loop limit and to size the `data_method` object.

```
if  ( method_setting >= 0 ) {
  { Int idr_table_len;
    Real**  idr_table = idr_get_real_table( parsed_data, method_setting,
                                            idr_table_len, 1, 1 );

    data_method.methodSetting.reshape(idr_table_len);
    for (int i = 0; i<idr_table_len; i++)
      data_method.methodSetting[i] = idr_table[0][i];
  }
}
```

Attention:

If no new data attributes have been added, but instead there are only new settings for existing attributes, then you're done with the database augmentation at this point (you just need to add code to use these new settings in the places where the existing attributes are used).

9.4.3 Augment/update get_<data_type>() functions

The final update step for ProblemDescDB.C involves extending the database retrieval functions. These retrieval functions accept an identifier string and return a database attribute of a particular type, e.g. a DakotaRealVector:

```
const DakotaRealVector& get_drv(const DakotaString& entry_name);
```

The implementation of each of these functions has a simple series of if-else checks which return the appropriate attribute based on the identifier string. For example,

```
if (entry_name == "variables.continuous_design.initial_point")
  return variablesList[variablesIndex].continuousDesignVars;
```

appears at the top of ProblemDescDB::get_drv(). Based on the identifier string, it returns the `continuousDesignVars` attribute from the DataVariables object. Since there may be multiple variables specifications, an index into a list of DataVariables objects is used. In particular, `variablesList` contains a list of all of the `data_variables` objects, one for each time `variables_kwhandler()` has been called by the parser. The particular variables object used for the data retrieval is managed by `variablesIndex`, which is set in a `set_db_list_nodes()` operation that will not be described here.

There may be multiple DataVariables, DataInterface, DataResponses, and/or DataMethod objects. However, only one strategy specification is currently allowed, so these specifications are handled with static attributes of the ProblemDescDB class rather than with a list (see also Update Corresponding Data Classes).

To augment the get_<data_type>() functions, add `else` blocks with new identifier strings which retrieve 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 `List[Index]` syntax for variables, interface, responses, and method specifications. For example, the `method_setting` example attribute would be added to `get_drv()` as:

```
else if (entry_name == "method.method_name.method_setting")
  return methodList[methodIndex].methodSetting;
```

A strategy specification addition would not use a `List[Index]` syntax, but would instead look like:

```
else if (entry_name == "strategy.strategy_name.strategy_setting")
  return strategySetting;
```

9.5 Update Corresponding Data Classes

In this step, we extend the Data class definitions to include the new attributes referenced in Update keyword handler logic blocks and Augment/update get_<data_type>() functions.

9.5.1 Update the Data class header file

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

9.5.2 Update the .C file

Define defaults for the new attributes in the constructor initialization list (or in the case of DataMethod, in the body of the constructor for readability). Add the new attributes to the assign() function for use by the copy constructor and assignment operator. Add the new attributes to the write(PackBuffer&), read(UnPackBuffer&), and write(ostream&) functions, paying attention to using a consistent ordering.

In the case of a strategy specification change, there is no DataStrategy container class since only one strategy specification is allowed and there is no need for a list of data objects. Rather, in this case, it is necessary to add static attributes to ProblemDescDB.H, add their initialization to the top of ProblemDescDB.C, and add them to the ProblemDescDB::send_db_buffer() and ProblemDescDB::receive_db_buffer() buffer insertion/extraction functions (again, paying attention to using a consistent ordering).

9.6 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, from DakotaModel.C:

```
const DakotaString& 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 indices (i.e., `methodIndex`, `interfaceIndex`, `variablesIndex`, and `responsesIndex`) 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.

9.7 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.input.spec** that have been modified should be updated.

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