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

Version 3.1 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

1 DAKOTA Developers Manual **11**

1.1 Introduction 11

1.2 Overview of DAKOTA 11

1.3 Services 15

1.4 Additional Resources 16

2 DAKOTA Hierarchical Index **17**

2.1 DAKOTA Class Hierarchy 17

3 DAKOTA Compound Index **21**

3.1 DAKOTA Compound List 21

4 DAKOTA File Index **25**

4.1 DAKOTA File List 25

5 DAKOTA Page Index **27**

5.1 DAKOTA Related Pages 27

6 DAKOTA Class Documentation **29**

6.1 AllMergedVarConstraints Class Reference 29

6.2 AllMergedVariables Class Reference 32

6.3 AllVarConstraints Class Reference 36

6.4 AllVariables Class Reference 39

6.5 AnalysisCode Class Reference 43

6.6 ANNSurf Class Reference 46

6.7 ApplicationInterface Class Reference 48

6.8 ApproximationInterface Class Reference 59

6.9 BaseConstructor Struct Reference 62

6.10 BranchBndStrategy Class Reference 63

6.11 COLINApplication Class Template Reference 65

6.12 COLINOptimizer Class Template Reference 68
6.13 ColinPoint Class Reference 70
6.14 CommandLineHandler Class Reference 71
6.15 CommandShell Class Reference 72
6.16 ConcurrentStrategy Class Reference 74
6.17 CONMINOptimizer Class Reference 76
6.18 CtelRegexp Class Reference 83
6.19 DACEIterator Class Reference 85
6.20 DakotaApproximation Class Reference 89
6.21 DakotaArray Class Template Reference 94
6.22 DakotaBaseVector Class Template Reference 98
6.23 DakotaBiStream Class Reference 102
6.24 DakotaBoStream Class Reference 105
6.25 DakotaGraphics Class Reference 108
6.26 DakotaInterface Class Reference 111
6.27 DakotaIterator Class Reference 117
6.28 DakotaLeastSq Class Reference 124
6.29 DakotaList Class Template Reference 126
6.30 DakotaMatrix Class Template Reference 130
6.31 DakotaModel Class Reference 132
6.32 DakotaNonD Class Reference 143
6.33 DakotaOptimizer Class Reference 147
6.34 DakotaOptLeastSq Class Reference 150
6.35 DakotaResponse Class Reference 154
6.36 DakotaResponseRep Class Reference 158
6.37 DakotaStrategy Class Reference 163
6.38 DakotaString Class Reference 169
6.39 DakotaVarConstraints Class Reference 172
6.40 DakotaVariables Class Reference 178
6.41 DakotaVector Class Template Reference 184
6.42 DataInterface Class Reference 188
6.43 DataMethod Class Reference 193
6.44 DataResponses Class Reference 200
6.45 DataStrategy Class Reference 203
6.46 DataVariables Class Reference 207
6.47 DirectFnApplicInterface Class Reference 212

6.48 DOTOptimizer Class Reference 216
6.49 ErrorTable Struct Reference 220
6.50 ForkAnalysisCode Class Reference 221
6.51 ForkApplicInterface Class Reference 223
6.52 FunctionCompare Class Template Reference 226
6.53 FundamentalVarConstraints Class Reference 227
6.54 FundamentalVariables Class Reference 231
6.55 GetLongOpt Class Reference 236
6.56 HermiteSurf Class Reference 240
6.57 HierLayeredModel Class Reference 242
6.58 KrigApprox Class Reference 246
6.59 KrigingSurf Class Reference 254
6.60 LayeredModel Class Reference 256
6.61 MARSSurf Class Reference 261
6.62 MergedVarConstraints Class Reference 263
6.63 MergedVariables Class Reference 266
6.64 MultilevelOptStrategy Class Reference 270
6.65 NestedModel Class Reference 273
6.66 NLSSOLLeastSq Class Reference 279
6.67 NoDBBaseConstructor Struct Reference 281
6.68 NonDAdvMeanValue Class Reference 282
6.69 NonDLHSSampling Class Reference 289
6.70 NonDOptStrategy Class Reference 291
6.71 NonDPCESampling Class Reference 293
6.72 NonDSampling Class Reference 295
6.73 NPSOLOptimizer Class Reference 298
6.74 ParallelLibrary Class Reference 301
6.75 ParamResponsePair Class Reference 313
6.76 ParamStudy Class Reference 316
6.77 ProblemDescDB Class Reference 320
6.78 RespSurf Class Reference 325
6.79 rSQPOptimizer Class Reference 327
6.80 SGOPTApplication Class Reference 329
6.81 SGOPTOptimizer Class Reference 332
6.82 SingleMethodStrategy Class Reference 335
6.83 SingleModel Class Reference 337

6.84 SNLLBase Class Reference . . . 339
6.85 SNLLLeastSq Class Reference . . . 342
6.86 SNLLOptimizer Class Reference . . . 345
6.87 SOLBase Class Reference . . . 350
6.88 SortCompare Class Template Reference . . . 353
6.89 SurrBasedOptStrategy Class Reference . . . 354
6.90 SurrLayeredModel Class Reference . . . 359
6.91 SurrogateDataPoint Class Reference . . . 364
6.92 SysCallAnalysisCode Class Reference . . . 366
6.93 SysCallApplicInterface Class Reference . . . 368
6.94 TaylorSurf Class Reference . . . 370
6.95 VariablesUtil Class Reference . . . 371

7 DAKOTA File Documentation 373

7.1 keywordtable.C File Reference . . . 373
7.2 main.C File Reference . . . 374
7.3 restart_util.C File Reference . . . 375

8 Interfacing with DAKOTA as a Library 379

8.1 Introduction . . . 379
8.2 Problem database populated through input file parsing . . . 380
8.3 Problem database populated through external means . . . 380
8.4 Performing an iterative study . . . 381
8.5 Retrieving data after a run . . . 381
8.6 Summary . . . 382

9 Performing Function Evaluations 383

9.1 Synchronous function evaluations . . . 383
9.2 Asynchronous function evaluations . . . 383
9.3 Analyses within each function evaluation . . . 384

10 Recommended Practices for DAKOTA Development 385

10.1 Introduction . . . 385
10.2 Style Guidelines . . . 385
10.3 File Naming Conventions . . . 387
10.4 Class Documentation Conventions . . . 388

11 Instructions for Modifying DAKOTA's Input Specification 389

11.1 Modify dakota.input.spec . . . 389

11.2 Rebuild IDR 390
11.3 Update keywordtable.C in $DAKOTA/src 390
11.4 Update ProblemDescDB.C in $DAKOTA/src 390
11.5 Update Corresponding Data Classes 393
11.6 Use get_<data_type>() Functions 394
11.7 Update the Documentation 394

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/main effects analysis with design of experiments and parameter study capabilities. 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 problem-solving environment as well as a platform for rapid prototyping of new solution approaches.

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

The 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 optimization iterator with a NestedModel. This NestedModel contains a sub-iterator and sub-model for performing uncertainty quantifications. 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 provides a base class for DOTOptimizer, CONMINOptimizer, NPSOLOptimizer, rSQPOptimizer, SNLLOptimizer, SGOPTOptimizer, and COLINOptimizer.
- Uncertainty quantification: DakotaNonD inherits from DakotaIterator and provides a base class for NonDAdvMeanValue and NonDSampling. NonDSampling is then further specialized with the NonDLHSSampling and NonDPCESampling derived classes.
- Parameter estimation: DakotaLeastSq provides a base class for SNLLLeastSq, a Gauss-Newton least squares solver, and NLSSOLLeastSq, an SQP-based least squares solver.
- Design of experiments: DACEIterator inherits directly from DakotaIterator. NonDLHSSampling from the uncertainty quantification branch also supports a design of experiments mode.
- 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 as part of every response evaluation on the top level model, but rather used periodically in surrogate update and verification steps.
- NestedModel: variables are mapped into responses using a combination of an optional 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 used to perform a complete iterative study as part of every response evaluation on the top level model.

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: both 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 (integrality is relaxed) for design, uncertain, and state variable types.
- AllMergedVariables: both 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 variables view that is chosen depends on the type of iterative study. For design optimization and uncertainty quantification, for example, variable and domain type distinctions are important and a FundamentalVariables view is used. For parameter studies and design of experiments, however, the variable type distinctions can be ignored and an AllVariables view is used. Finally, the branch and bound strategy relies on relaxation of integrality so that continuous optimizers may be used for mixed integer problems. In this case, a MergedVariables view is used.

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.
- GridApplicInterface: the simulation is invoked using distributed resource facilities. This capability is experimental and still under development. The design is evolving into the use of Condor and/or Globus tools.

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 data fit 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).

Note: in the data fit approximation case, SurrLayeredModel provides the bulk of the surrogate management logic. It contains an ApproximationInterface object which provides the approximate parameter to response mappings. In the hierarchical approximation case, an ApproximationInterface object is not used since HierLayeredModel contains low and high fidelity application interfaces.

1.2.6 Responses

Class: DakotaResponse.

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

1.3 Services

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

- 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 manages concurrent analyses executing on multiple processors. Partitioning of these levels with MPI communicators is managed in ParallelLibrary and scheduling routines for the levels are part of 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 ProblemDescDB::manage_inputs() called from main.C. IDR populates data within the ProblemDescDB support class, which maintains a DataStrategy specification and lists of DataMethod, DataVariables, DataInterface, and DataResponses specifications. Procedures for modifying the parsing subsystem are described in Instructions for Modifying DAKOTA's Input Specification.
- Failure capturing: Simulation failures can be trapped and managed using exception handling in ApplicationInterface and its derived classes.
- Restart: DAKOTA maintains a record of all function evaluations both in memory (for capturing any duplication) and on the file system (for restarting runs). Restart options are processed in CommandLineHandler, restart file management occurs in ParallelLibrary::manage_outputs_restart() called from 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 data-intensive classes which do not involve a class hierarchy. Currently, only the DakotaResponse class uses this idiom.
- Graphics: DAKOTA provides 2D iteration history graphics using Motif widgets and 3D surface plotting 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.

1.4 Additional Resources

Additional development resources include:

- Recommended Practices for DAKOTA Development
- Instructions for Modifying DAKOTA's Input Specification
- 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 these evaluations is provided in Performing Function Evaluations.
- In addition to its normal usage as a stand-alone application, DAKOTA may be interfaced as an algorithm library as described in Interfacing with DAKOTA as a Library.
- 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:

- AnalysisCode . . . 43
  - ForkAnalysisCode . . . 221
  - SysCallAnalysisCode . . . 366
- BaseConstructor . . . 62
- COLINApplication< DomainT, ResponseT > . . . 65
- ColinPoint . . . 70
- CommandShell . . . 72
- CtelRegexp . . . 83
- DakotaApproximation . . . 89
  - ANNSurf . . . 46
  - HermiteSurf . . . 240
  - KrigingSurf . . . 254
  - MARSSurf . . . 261
  - RespSurf . . . 325
  - TaylorSurf . . . 370
- DakotaArray< T > . . . 94
- DakotaBaseVector< T > . . . 98
  - DakotaVector< T > . . . 184
- DakotaBaseVector< DakotaBaseVector< T > > . . . 98
  - DakotaMatrix< T > . . . 130
- DakotaBiStream . . . 102
- DakotaBoStream . . . 105
- DakotaGraphics . . . 108
- DakotaInterface . . . 111
  - ApplicationInterface . . . 48
    - DirectFnApplicInterface . . . 212
    - ForkApplicInterface . . . 223
    - SysCallApplicInterface . . . 368
  - ApproximationInterface . . . 59
- DakotaIterator . . . 117
  - DACEIterator . . . 85

DakotaNonD . . . 143
NonDAdvMeanValue . . . 282
NonDSampling . . . 295
NonDLHSSampling . . . 289
NonDPCESampling . . . 293
DakotaOptLeastSq . . . 150
DakotaLeastSq . . . 124
NLSSOLLeastSq . . . 279
SNLLLeastSq . . . 342
DakotaOptimizer . . . 147
COLINOptimizer< OptimizerT > . . . 68
CONMINOptimizer . . . 76
DOTOptimizer . . . 216
NPSOLOptimizer . . . 298
rSQPOptimizer . . . 327
SGOPTOptimizer . . . 332
SNLLOptimizer . . . 345
ParamStudy . . . 316
DakotaList< T > . . . 126
DakotaModel . . . 132
LayeredModel . . . 256
HierLayeredModel . . . 242
SurrLayeredModel . . . 359
NestedModel . . . 273
SingleModel . . . 337
DakotaResponse . . . 154
DakotaResponseRep . . . 158
DakotaStrategy . . . 163
BranchBndStrategy . . . 63
ConcurrentStrategy . . . 74
MultilevelOptStrategy . . . 270
NonDOptStrategy . . . 291
SingleMethodStrategy . . . 335
SurrBasedOptStrategy . . . 354
DakotaString . . . 169
DakotaVarConstraints . . . 172
AllMergedVarConstraints . . . 29
AllVarConstraints . . . 36
FundamentalVarConstraints . . . 227
MergedVarConstraints . . . 263
DakotaVariables . . . 178
AllMergedVariables . . . 32
AllVariables . . . 39
FundamentalVariables . . . 231
MergedVariables . . . 266
DataInterface . . . 188
DataMethod . . . 193
DataResponses . . . 200
DataStrategy . . . 203
DataVariables . . . 207
ErrorTable . . . 220
FunctionCompare< T > . . . 226

GetLongOpt 236
- CommandLineHandler 71

KrigApprox 246
NoDBBaseConstructor 281
ParallelLibrary 301
ParamResponsePair 313
ProblemDescDB 320
SGOPTApplication 329
SNLLBase 339
- SNLLLeastSq 342
- SNLLOptimizer 345

SOLBase 350
- NLSSOLLeastSq 279
- NPSOLOptimizer 298

SortCompare< T > 353
SurrogateDataPoint 364
VariablesUtil 371
- AllMergedVarConstraints 29
- AllMergedVariables 32
- AllVarConstraints 36
- AllVariables 39
- FundamentalVarConstraints 227
- FundamentalVariables 231
- MergedVarConstraints 263
- MergedVariables 266

Chapter 3

DAKOTA Compound Index

3.1 DAKOTA Compound List

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

AllMergedVarConstraints (Derived class within the DakotaVarConstraints hierarchy which combines the all and merged data views) 29
AllMergedVariables (Derived class within the DakotaVariables hierarchy which combines the all and merged data views) 32
AllVarConstraints (Derived class within the DakotaVarConstraints hierarchy which employs the all data view) 36
AllVariables (Derived class within the DakotaVariables hierarchy which employs the all data view) 39
AnalysisCode (Base class providing common functionality for derived classes (SysCallAnalysisCode and ForkAnalysisCode) which spawn separate processes for managing simulations) 43
ANNSurf (Derived approximation class for artificial neural networks) 46
ApplicationInterface (Derived class within the interface class hierarchy for supporting interfaces to simulation codes) 48
ApproximationInterface (Derived class within the interface class hierarchy for supporting approximations to simulation-based results) 59
BaseConstructor (Dummy struct for overloading letter-envelope constructors) 62
BranchBndStrategy (Strategy for mixed integer nonlinear programming using the PICO parallel branch and bound engine) 63
COLINApplication< DomainT, ResponseT > 65
COLINOptimizer< OptimizerT > (Wrapper class for optimizers defined using COLIN) 68
ColinPoint 70
CommandLineHandler (Utility class for managing command line inputs to DAKOTA) 71
CommandShell (Utility class which defines convenience operators for spawning processes with system calls) 72
ConcurrentStrategy (Strategy for multi-start iteration or pareto set optimization) 74
CONMINOptimizer (Wrapper class for the CONMIN optimization library) 76
CtelRegexp 83
DACEIterator (Wrapper class for the DDACE design of experiments library) 85
DakotaApproximation (Base class for the approximation class hierarchy) 89
DakotaArray< T > (Template class for the Dakota bookkeeping array) 94
DakotaBaseVector< T > (Base class for the DakotaMatrix and DakotaVector classes) 98
DakotaBiStream (The binary input stream class. Overloads the >> operator for all data types) . 102
DakotaBoStream (The binary output stream class. Overloads the << operator for all data types) 105

DakotaGraphics (Single interface to 2D (motif) and 3D (PLPLOT) graphics as well as tabular cataloguing of data for post-processing with Matlab, Tecplot, etc) 108
DakotaInterface (Base class for the interface class hierarchy) 111
DakotaIterator (Base class for the iterator class hierarchy) 117
DakotaLeastSq (Base class for the nonlinear least squares branch of the iterator hierarchy) . . . 124
DakotaList< T > (Template class for the Dakota bookkeeping list) 126
DakotaMatrix< T > (Template class for the Dakota numerical matrix) 130
DakotaModel (Base class for the model class hierarchy) 132
DakotaNonD (Base class for all nondetermistic iterators (the DAKOTA/UQ branch)) 143
DakotaOptimizer (Base class for the optimizer branch of the iterator hierarchy) 147
DakotaOptLeastSq (Base class for the optimizer and least squares branches of the iterator hierarchy) 150
DakotaResponse (Container class for response functions and their derivatives. DakotaResponse provides the handle class) 154
DakotaResponseRep (Container class for response functions and their derivatives. Dakota-ResponseRep provides the body class) 158
DakotaStrategy (Base class for the strategy class hierarchy) 163
DakotaString (DakotaString class, used as main string class for Dakota) 169
DakotaVarConstraints (Base class for the variable constraints class hierarchy) 172
DakotaVariables (Base class for the variables class hierarchy) 178
DakotaVector< T > (Template class for the Dakota numerical vector) 184
DataInterface (Container class for interface specification data) 188
DataMethod (Container class for method specification data) 193
DataResponses (Container class for responses specification data) 200
DataStrategy (Container class for strategy specification data) 203
DataVariables (Container class for variables specification data) 207
DirectFnApplicInterface (Derived application interface class which spawns simulation codes and testers using direct procedure calls) 212
DOTOptimizer (Wrapper class for the DOT optimization library) 216
ErrorTable (Data structure to hold errors) 220
ForkAnalysisCode (Derived class in the AnalysisCode class hierarchy which spawns simulations using forks) 221
ForkApplicInterface (Derived application interface class which spawns simulation codes using forks) 223
FunctionCompare< T > 226
FundamentalVarConstraints (Derived class within the DakotaVarConstraints hierarchy which employs the default data view (no variable or domain type array merging)) 227
FundamentalVariables (Derived class within the DakotaVariables hierarchy which employs the default data view (no variable or domain type array merging)) 231
GetLongOpt (GetLongOpt is a general command line utility from S. Manoharan (Advanced Computer Research Institute, Lyon, France)) 236
HermiteSurf (Derived approximation class for Hermite polynomials (global approximation)) . . 240
HierLayeredModel (Derived model class within the layered model branch for managing hierarchical surrogates (models of varying fidelity)) 242
KrigApprox (Utility class for kriging interpolation) 246
KrigingSurf (Derived approximation class for kriging interpolation) 254
LayeredModel (Base class for the layered models (SurrLayeredModel and HierLayeredModel)) 256
MARSSurf (Derived approximation class for multivariate adaptive regression splines) 261
MergedVarConstraints (Derived class within the DakotaVarConstraints hierarchy which employs the merged data view) 263
MergedVariables (Derived class within the DakotaVariables hierarchy which employs the merged data view) 266
MultilevelOptStrategy (Strategy for hybrid optimization using multiple optimizers on multiple models of varying fidelity) 270

NestedModel (Derived model class which performs a complete sub-iterator execution within every evaluation of the model) . . . 273
NLSSOLLeastSq (Wrapper class for the NLSSOL nonlinear least squares library) . . . 279
NoDBBaseConstructor (Dummy struct for overloading constructors used in on-the-fly instantiations) . . . 281
NonDAdvMeanValue (Class for the analytical reliability methods within DAKOTA/UQ) . . . 282
NonDLHSSampling (Performs LHS and Monte Carlo sampling for uncertainty quantification) . 289
NonDOptStrategy (Strategy for optimization under uncertainty (robust and reliability-based design)) . . . 291
NonDPCESampling (Stochastic finite element approach to uncertainty quantification using polynomial chaos expansions) . . . 293
NonDSampling (Base class for common code between NonDLHSSampling and NonDPCESampling) . . . 295
NPSOLOptimizer (Wrapper class for the NPSOL optimization library) . . . 298
ParallelLibrary (Class for managing partitioning of multiple levels of parallelism and message passing within the levels) . . . 301
ParamResponsePair (Container class for a variables object, a response object, and an evaluation id) 313
ParamStudy (Class for vector, list, centered, and multidimensional parameter studies) . . . 316
ProblemDescDB (The database containing information parsed from the DAKOTA input file) . . 320
RespSurf (Derived approximation class for polynomial regression) . . . 325
rSQPOptimizer . . . 327
SGOPTApplication (Maps the evaluation functions used by SGOPT algorithms to the DAKOTA evaluation functions) . . . 329
SGOPTOptimizer (Wrapper class for the SGOPT optimization library) . . . 332
SingleMethodStrategy (Simple fall-through strategy for running a single iterator on a single model) 335
SingleModel (Derived model class which utilizes a single interface to map variables into responses) 337
SNLLBase (Base class for OPT++ optimization and least squares methods) . . . 339
SNLLLeastSq (Wrapper class for the OPT++ optimization library) . . . 342
SNLLOptimizer (Wrapper class for the OPT++ optimization library) . . . 345
SOLBase (Base class for Stanford SOL software) . . . 350
SortCompare< T > . . . 353
SurrBasedOptStrategy (Strategy for provably-convergent surrogate-based optimization) . . . 354
SurrLayeredModel (Derived model class within the layered model branch for managing data fit surrogates (global and local)) . . . 359
SurrogateDataPoint (Simple container class encapsulating basic parameter and response data for defining a "truth" data point) . . . 364
SysCallAnalysisCode (Derived class in the AnalysisCode class hierarchy which spawns simulations using system calls) . . . 366
SysCallApplicInterface (Derived application interface class which spawns simulation codes using system calls) . . . 368
TaylorSurf (Derived approximation class for 1st order Taylor series (local approximation)) . . . 370
VariablesUtil (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) . . . 371

Chapter 4

DAKOTA File Index

4.1 DAKOTA File List

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

keywordtable.C (File containing keywords for the strategy, method, variables, interface, and responses input specifications from **dakota.input.spec**) 373
main.C (File containing the main program for DAKOTA) 374
restart_util.C (File containing the DAKOTA restart utility main program) 375

Chapter 5

DAKOTA Page Index

5.1 DAKOTA Related Pages

Here is a list of all related documentation pages:

Interfacing with DAKOTA as a Library 379
Performing Function Evaluations 383
Recommended Practices for DAKOTA Development 385
Instructions for Modifying DAKOTA's Input Specification 389

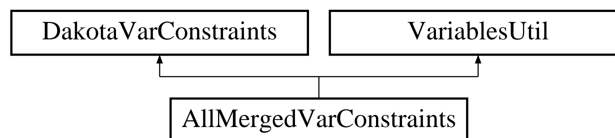
Chapter 6

DAKOTA Class Documentation

6.1 AllMergedVarConstraints Class Reference

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

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.
- const DakotaRealVector & inactive_continuous_lower_bounds () const
  return the inactive continuous lower bounds.
- void inactive_continuous_lower_bounds (const DakotaRealVector &i_c_l_bnds)
  set the inactive continuous lower bounds.
- const DakotaRealVector & inactive_continuous_upper_bounds () const
  return the inactive continuous upper bounds.
- void inactive_continuous_upper_bounds (const DakotaRealVector &i_c_u_bnds)
  set the inactive continuous upper bounds.
- const DakotaIntVector & inactive_discrete_lower_bounds () const
  return the inactive discrete lower bounds.
- void inactive_discrete_lower_bounds (const DakotaIntVector &i_d_l_bnds)
  set the inactive discrete lower bounds.
- const DakotaIntVector & inactive_discrete_upper_bounds () const
  return the inactive discrete upper bounds.
- void inactive_discrete_upper_bounds (const DakotaIntVector &i_d_u_bnds)
  set the inactive discrete upper bounds.
- DakotaRealVector all_continuous_lower_bounds () const
  returns a single array with all continuous lower bounds.
- DakotaRealVector all_continuous_upper_bounds () const
  returns a single array with all continuous upper bounds.
- DakotaIntVector all_discrete_lower_bounds () const
  returns a single array with all discrete lower bounds.
- DakotaIntVector all_discrete_upper_bounds () const
  returns a single array with all discrete 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.

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.

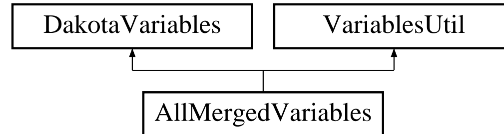
The documentation for this class was generated from the following files:

- AllMergedVarConstraints.H
- AllMergedVarConstraints.C

6.2 AllMergedVariables Class Reference

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

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.
- DakotaStringArray all_continuous_variable_labels () const
  returns a single array with all continuous variable labels.
- DakotaStringArray all_discrete_variable_labels () const
  returns a single array with all discrete variable labels.
- 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.

Friends

- bool 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.

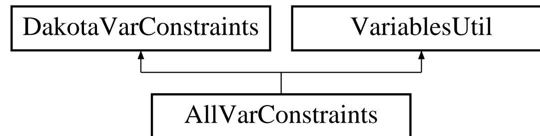
The documentation for this class was generated from the following files:

- AllMergedVariables.H
- AllMergedVariables.C

6.3 AllVarConstraints Class Reference

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

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.

- const DakotaRealVector & inactive_continuous_lower_bounds () const

  return the inactive continuous lower bounds.

- void inactive_continuous_lower_bounds (const DakotaRealVector &i_c_l_bnds)
  set the inactive continuous lower bounds.
- const DakotaRealVector & inactive_continuous_upper_bounds () const
  return the inactive continuous upper bounds.
- void inactive_continuous_upper_bounds (const DakotaRealVector &i_c_u_bnds)
  set the inactive continuous upper bounds.
- const DakotaIntVector & inactive_discrete_lower_bounds () const
  return the inactive discrete lower bounds.
- void inactive_discrete_lower_bounds (const DakotaIntVector &i_d_l_bnds)
  set the inactive discrete lower bounds.
- const DakotaIntVector & inactive_discrete_upper_bounds () const
  return the inactive discrete upper bounds.
- void inactive_discrete_upper_bounds (const DakotaIntVector &i_d_u_bnds)
  set the inactive discrete upper bounds.
- DakotaRealVector all_continuous_lower_bounds () const
  returns a single array with all continuous lower bounds.
- DakotaRealVector all_continuous_upper_bounds () const
  returns a single array with all continuous upper bounds.
- DakotaIntVector all_discrete_lower_bounds () const
  returns a single array with all discrete lower bounds.
- DakotaIntVector all_discrete_upper_bounds () const
  returns a single array with all discrete 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.

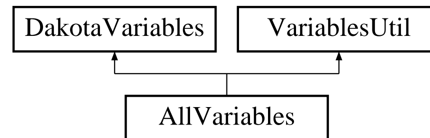
The documentation for this class was generated from the following files:

- AllVarConstraints.H
- AllVarConstraints.C

6.4 AllVariables Class Reference

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

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.

- DakotaStringArray all_continuous_variable_labels () const

  returns a single array with all continuous variable labels.

- DakotaStringArray all_discrete_variable_labels () const

  returns a single array with all discrete variable labels.

- 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).

- 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

- bool 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.

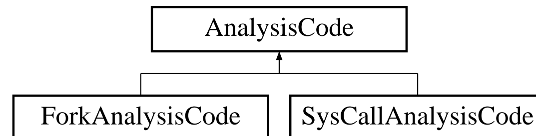
The documentation for this class was generated from the following files:

- 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.

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 suppress_output_flag (const bool flag)

  set suppressOutputFlag.

- bool suppress_output_flag () const

  return suppressOutputFlag.

Protected Methods

- AnalysisCode (const ProblemDescDB &problem_db)

    constructor.

- virtual ~AnalysisCode ()

    destructor.

Protected Attributes

- bool suppressOutputFlag

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

- bool verboseFlag

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

- bool fileTagFlag

    flags tagging of parameter/results files.

- bool fileSaveFlag

    flags retention of parameter/results files.

- bool 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.

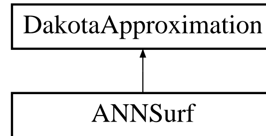
The documentation for this class was generated from the following files:

- AnalysisCode.H
- AnalysisCode.C

6.6 ANNSurf Class Reference

Derived approximation class for artificial neural networks.

Inheritance diagram for ANNSurf::



Public Methods

- ANNSurf (const ProblemDescDB &problem_db, const size_t &num_acv)

  constructor.

- ~ANNSurf ()

  destructor.

Protected Methods

- int required_samples ()

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

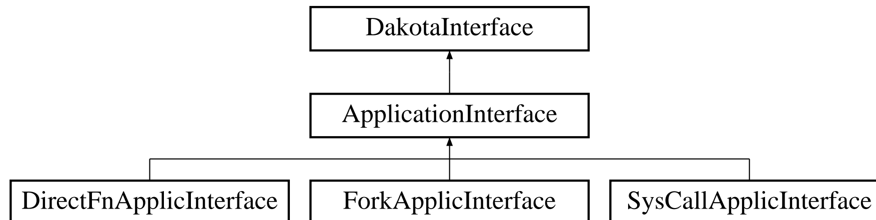
The documentation for this class was generated from the following files:

- ANNSurf.H
- ANNSurf.C

6.7 ApplicationInterface Class Reference

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

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

- void free_communicators ()

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

- void init_serial ()
- 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 bool 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 DakotaResponseArray & synch ()

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

- const DakotaResponseList & 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 (DakotaPRPList &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 (DakotaPRPList &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.

- bool evalMessagePass

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

- bool analysisMessagePass

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

- bool 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.

- bool 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.

- bool evalDedMasterFlag

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

- bool 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.

- MPI_Comm evalAnalysisIntraComm

  intracomm for all analysisCommRank==0 within 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

- bool duplication_detect (const DakotaVariables &vars, DakotaResponse &response, const bool 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 (DakotaPRPList &prp_list)

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

- void synchronous_local_evaluations (DakotaPRPList &prp_list)

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

- void asynchronous_local_evaluations_nowait (DakotaPRPList &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.

- bool headerFlag

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

- bool asvControlFlag

  used to manage a user request to deactivate the active set vector control. true = modify the ASV each evaluation as appropriate (default); false = ASV values are static so that the user need not check them on each evaluation.

- bool evalCacheFlag

  used to manage a user request to deactivate the function evaluation cache (i.e., queries and insertions using the data_pairs list).

- bool restartFileFlag

  used to manage a user request to deactivate the restart file (i.e., insertions into write_restart).

- 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.

- DakotaResponseList 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.

- DakotaResponseList 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.

- DakotaPRPList 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 distributed resource facilities.

6.7.2 Member Function Documentation

6.7.2.1 void ApplicationInterface::init_serial () `[protected, virtual]`

DataInterface.C defaults of 0 servers are needed to distinguish an explicit user request for 1 server (serialization of a parallelism level) from no user request (use parallel auto-config). This default causes problems when init_communicators() is not called for an interface object (e.g., static scheduling fails in DirectFnApplicInterface::derived_map() for NestedModel::optionalInterface). This is the reason for this function: to reset certain defaults for interface objects that are used serially.

Reimplemented from DakotaInterface.

6.7.2.2 void ApplicationInterface::map (const DakotaVariables & *vars*, const DakotaIntArray & *asv*, DakotaResponse & *response*, const bool *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.

6.7.2.3 const DakotaResponseArray & 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.

6.7.2.4 const DakotaResponseList & 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.

6.7.2.5 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.

6.7.2.6 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.

6.7.2.7 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.

6.7.2.8 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().

6.7.2.9 bool ApplicationInterface::duplication_detect (const DakotaVariables & *vars*, DakotaResponse & *response*, const bool *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(). Note that the list searches can get very expensive if a long list is searched on every new function evaluation (either from a large number of previous jobs, a large number of pending jobs, or both). For this reason, a user request for deactivation of the evaluation cache results in a complete bypass of duplication_detect(), even though a beforeSynchPRPList search would still be meaningful. Since the intent of this request is to streamline operations, both list searches are bypassed.

6.7.2.10 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.

6.7.2.11 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.

6.7.2.12 void ApplicationInterface::asynchronous_local_evaluations (DakotaPRPList & *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, non-blocking 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()).

6.7.2.13 void ApplicationInterface::synchronous_local_evaluations (DakotaPRPList & *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.

6.7.2.14 void ApplicationInterface::asynchronous_local_evaluations_nowait (DakotaPRPList & *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().

6.7.2.15 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()).

6.7.2.16 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).

6.7.2.17 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 either the bcast() in synchronous_local_evaluations(), which is invoked by static_schedule_evaluations()), or the bcast() in map().

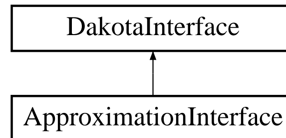
The documentation for this class was generated from the following files:

- ApplicationInterface.H
- ApplicationInterface.C

6.8 ApproximationInterface Class Reference

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

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 bool 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, const DakotaRealVector &lower_bnds, const DakotaRealVector &upper_bnds)

  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 DakotaRealVectorArray & approximation_coefficients ()

  retrieve the approximation coefficients from each DakotaApproximation within an ApproximationInterface.

- const DakotaResponseArray & synch ()

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

- const DakotaResponseList & 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.

- DakotaRealVectorArray functionSurfaceCoeffs

  array of approximation coefficient vectors, one vector per response function.

- DakotaString sampleReuse

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

- DakotaString sampleReuseFile

  file name for sampleReuse == "file".

- bool graphicsFlag

  controls 3D graphics of approximation surfaces.

- int minSamples

  the minimum number of samples over all functionSurfaces.

- DakotaResponseList 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.

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.

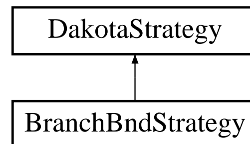
The documentation for this struct was generated from the following file:

- ProblemDescDB.H

6.10 BranchBndStrategy Class Reference

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

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 COLINApplication Class Template Reference

Public Methods

- COLINApplication (DakotaModel &model, DakotaResponse(∗multiobj_mod_ptr)(const DakotaResponse &))

  destructor.

- **∼COLINApplication** ()
- void DoEval (DomainT &point, ResponseT ∗response, bool synch_flag)

  launch a function evaluation either synchronously or asynchronously.

- void synchronize ()

  blocking retrieval of all pending jobs.

- void next_eval (int &id)

  nonblocking query and retrieval of a job if completed.

- void dakota_asynch_flag (const bool &asynch_flag)

  Try to terminate a function evaluation TODO: supported by DAKOTA?

Private Methods

- void map_response (ResponseT &colin_response, const DakotaResponse &dakota_response)

Private Attributes

- DakotaModel & userDefinedModel

  reference to the COLINOptimizer's model passed in the constructor.

- DakotaIntArray activeSetVector

  copy/conversion of the COLIN request vector.

- bool dakotaModelAsynchFlag

  a flag for asynchronous DAKOTA evaluations.

- DakotaResponseList 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.

- int **num_real_params**
- int **num_integer_params**
- DakotaVariables **dakota_vars**

6.11.1 Detailed Description

template<class DomainT, class ResponseT> class COLINApplication< DomainT, ResponseT >

COLINApplication is a DAKOTA class that is derived from COLIN's OptApplication hierarchy. It redefines a variety of virtual COLIN functions to use the corresponding DAKOTA functions. This is a more flexible algorithm library interfacing approach than can be obtained with the function pointer approaches used by NPSOLOptimizer and SNLLOptimizer.

6.11.2 Member Function Documentation

6.11.2.1 template<class DomainT, class ResponseT> void COLINApplication< DomainT, ResponseT >::DoEval (DomainT & *pt*, ResponseT ∗ *prob_response*, bool *synch_flag*)

launch a function evaluation either synchronously or asynchronously.

Converts the DomainT 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 ResponseT response (synchronous) or bookkeeps the response object (asynchronous).

6.11.2.2 template<class DomainT, class ResponseT> void COLINApplication< DomainT, ResponseT >::synchronize ()

blocking retrieval of all pending jobs.

Blocking synchronize of asynchronous DAKOTA jobs followed by conversion of the DakotaResponse objects to ResponseT response objects.

6.11.2.3 template<class DomainT, class ResponseT> void COLINApplication< DomainT, ResponseT >::next_eval (int & *id*)

nonblocking query and retrieval of a job if completed.

Nonblocking job retrieval. Finds a completion (if available), populates the COLIN response, and sets id to the completed job's id. Else set id = -1.

6.11.2.4 template<class DomainT, class ResponseT> void COLINApplication< DomainT, ResponseT >::dakota_asynch_flag (const bool & *asynch_flag*) [inline]

Try to terminate a function evaluation TODO: supported by DAKOTA?

This function is needed to publish the iterator's asynchFlag at run time (asynchFlag not available at construction).

6.11.2.5 template<class DomainT, class ResponseT> void COLINApplication< DomainT, ResponseT >::map_response (ResponseT & *colin_response*, const DakotaResponse & *dakota_response*) [private]

map_response Maps a DakotaResponse object into a ResponseT class that is compatable with COLIN.

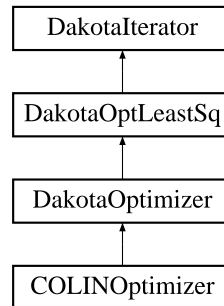
The documentation for this class was generated from the following file:

- COLINApplication.H

6.12 COLINOptimizer Class Template Reference

Wrapper class for optimizers defined using COLIN.

Inheritance diagram for COLINOptimizer::



Public Methods

- COLINOptimizer (DakotaModel &model)

  constructor.

- ~COLINOptimizer ()

  destructor.

- void find_optimum ()

  Performs the iterations to determine the optimal solution.

Protected Methods

- virtual void **set_rng** ()
- virtual void **set_initial_point** (ColinPoint &pt)
- virtual void **get_min_point** (ColinPoint &pt)
- virtual void set_method_options ()

  sets options for the methods based on user specifications.

- void set_standard_method_options ()

Protected Attributes

- OptimizerT * optimizer

  Pointer to COLIN base optimizer object.

- OptProblem< ColinPoint > problem

  pointer to COLIN problem object.

- RNG * rng

  RNG ptr.

6.12.1 Detailed Description

template<class OptimizerT> class COLINOptimizer< OptimizerT >

Wrapper class for optimizers defined using COLIN.

The COLINOptimizer class provides a templated wrapper for COLIN, a Sandia-developed C++ optimization interface library. A variety of COLIN optimizers are defined in the COLINY optimization library, which contains the optimization components from the old SGOPT library. COLINY contains optimizers such as genetic algorithms, pattern search methods, and other nongradient-based techniques. COLINOptimizer uses a COLINApplication object to perform the function evaluations.

The user input mappings are as follows: `max_iterations`, `max_function_evaluations`, `convergence_tolerance`, `solution_accuracy` and `max_cpu_time` are mapped into COLIN's `max_iters`, `max_neval`, `ftol`, `accuracy`, and `max_time` data attributes. An `output` setting of `verbose` is passed to COLIN's set_output() function and a setting of `debug` activates output of method initialization and sets the COLIN `debug` attribute to 10000. COLIN 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 COLINApplication 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 COLIN objects and controls.

6.12.2 Member Function Documentation

6.12.2.1 template<class OptimizerT> void COLINOptimizer< OptimizerT >::find_optimum () `[virtual]`

Performs the iterations to determine the optimal solution.

find_optimum redefines the DakotaOptimizer virtual function to perform the optimization using COLIN. It first sets up the problem data, then executes minimize() on the COLIN optimizer, and finally catalogues the results.

Implements DakotaOptimizer.

6.12.2.2 template<class OptimizerT> void COLINOptimizer< OptimizerT >::set_standard_method_options () `[protected]`

set_standard_method_options propagates standard DAKOTA user input to the optimizer.

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

- COLINOptimizer.H

6.13 ColinPoint Class Reference

Public Attributes

- vector< double > **rvec**
- vector< int > **ivec**

6.13.1 Detailed Description

A class containing a vector of doubles and integers.

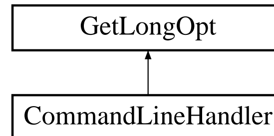
The documentation for this class was generated from the following file:

- COLINOptimizer.H

6.14 CommandLineHandler Class Reference

Utility class for managing command line inputs to DAKOTA.

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.

- int read_restart_evals () const

  Returns the number of evaluations to be read from the restart file (as specified on the DAKOTA command line) as an integer instead of a const char.*

6.14.1 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

6.15 CommandShell Class Reference

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

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 bool flag)

  set the asynchFlag.

- bool asynch_flag () const

  get the asynchFlag.

- void suppress_output_flag (const bool flag)

  set the suppressOutputFlag.

- bool suppress_output_flag () const

  get the suppressOutputFlag.

Private Attributes

- DakotaString unixCommand

  the command string that is constructed through one or more << insertions and then executed by flush.

- bool asynchFlag

  flags nonblocking operation (background system calls).

- bool suppressOutputFlag

  flags suppression of shell output (no command echo).

6.15.1 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.

6.15.2 Member Function Documentation

6.15.2.1 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 suppressOutputFlag is not set.

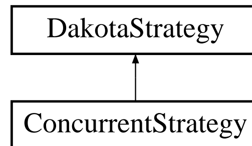
The documentation for this class was generated from the following files:

- CommandShell.H
- CommandShell.C

6.16 ConcurrentStrategy Class Reference

Strategy for multi-start iteration or pareto set optimization.

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 parameterSets

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

- bool multiStartFlag

  a flag for distinguishing multi-start from Pareto set.

- bool strategyDedicatedMasterFlag

  signals ded. master partitioning.

- int iteratorServerId

  identifier for an iterator server.

6.16.1 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.

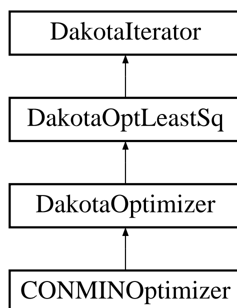
The documentation for this class was generated from the following files:

- ConcurrentStrategy.H
- ConcurrentStrategy.C

6.17 CONMINOptimizer Class Reference

Wrapper class for the CONMIN optimization library.

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.

6.17.1 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.

6.17.2 Member Data Documentation

6.17.2.1 int CONMINOptimizer::conminInfo `[private]`

INFO from CONMIN manual.

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

6.17.2.2 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

6.17.2.3 int CONMINOptimizer::optimizationType `[private]`

MINMAX from DOT manual (minimize or maximize).

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

6.17.2.4 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).

6.17.2.5 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.

6.17.2.6 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.

6.17.2.7 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.

6.17.2.8 int CONMINOptimizer::N1 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

N1 = number of variables + 2

6.17.2.9 int CONMINOptimizer::N2 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

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

6.17.2.10 int CONMINOptimizer::N3 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

N3 = Maximum possible number of active constraints.

6.17.2.11 int CONMINOptimizer::N4 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

N4 = Maximum(N3,number of variables)

6.17.2.12 int CONMINOptimizer::N5 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

N5 = 2*(N4)

6.17.2.13 Real CONMINOptimizer::CT `[private]`

Constraint thickness parameter.

The value of CT decreases in magnitude during optimization.

6.17.2.14 Real* CONMINOptimizer::S `[private]`

Internal CONMIN array.

Move direction in N-dimensional space.

6.17.2.15 Real* CONMINOptimizer::G1 `[private]`

Internal CONMIN array.

Temporary storage of constraint values.

6.17.2.16 Real* CONMINOptimizer::G2 `[private]`

Internal CONMIN array.

Temporary storage of constraint values.

6.17.2.17 Real* CONMINOptimizer::B `[private]`

Internal CONMIN array.

Temporary storage for computations involving array S.

6.17.2.18 Real* CONMINOptimizer::C `[private]`

Internal CONMIN array.

Temporary storage for use with arrays B and S.

6.17.2.19 int* CONMINOptimizer::MS1 `[private]`

Internal CONMIN array.

Temporary storage for use with arrays B and S.

6.17.2.20 Real* CONMINOptimizer::SCAL `[private]`

Internal CONMIN array.

Vector of scaling parameters for design parameter values.

6.17.2.21 Real* CONMINOptimizer::DF [private]

Internal CONMIN array.

Temporary storage for analytic gradient data.

6.17.2.22 Real* CONMINOptimizer::A [private]

Internal CONMIN array.

Temporary 2-D array for storage of constraint gradients.

6.17.2.23 int* CONMINOptimizer::ISC [private]

Internal CONMIN array.

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

6.17.2.24 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

6.18 CtelRegexp Class Reference

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.

6.18.1 Detailed Description

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

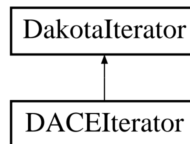
The documentation for this class was generated from the following files:

- CtelRegExp.H
- CtelRegExp.C

6.19 DACEIterator Class Reference

Wrapper class for the DDACE design of experiments library.

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, bool all_data_flag, bool 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, central_composite, 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).

- const int originalSeed

  the user seed specification for the random number generator (allows repeatable results).

- int randomSeed

  current seed for the random number generator.

- bool allDataFlag

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

- size_t numDACERuns

  counter for number of executions of run_iterator() for this object.

- bool varyPattern

  flag for continuing the random number sequence from a previous run_iterator() execution (e.g., for surrogate-based optimization) so that multiple executions are repeatable but not correlated.

- 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.

6.19.1 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.

6.19.2 Constructor & Destructor Documentation

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

primary constructor for building a standard iterator.

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

6.19.2.2 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.

6.19.3 Member Function Documentation

6.19.3.1 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.

6.19.3.2 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.

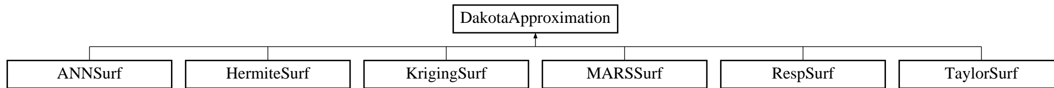
The documentation for this class was generated from the following files:

- DACEIterator.H
- DACEIterator.C

6.20 DakotaApproximation Class Reference

Base class for the approximation class hierarchy.

Inheritance diagram for DakotaApproximation::



Public Methods

- DakotaApproximation ()

  default constructor.

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

  standard constructor for envelope.

- DakotaApproximation (const DakotaApproximation &approx)

  copy constructor.

- virtual ~DakotaApproximation ()

  destructor.

- DakotaApproximation operator= (const DakotaApproximation &approx)

  assignment operator.

- 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 ()

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

- virtual const DakotaRealVector & approximation_coefficients ()

  return the coefficient array computed by find_coefficients().

- void build (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).

- int num_variables () const

  return the number of variables used in the approximation.

Protected Methods

- DakotaApproximation (BaseConstructor, const ProblemDescDB &problem_db, const size_t &num_-acv)

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

- virtual void find_coefficients ()

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

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.

- bool gradientFlag

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

- bool verboseFlag

  flag for verbose approximation output.

- 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, const size_t &num_acv)

  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.

6.20.1 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.

6.20.2 Constructor & Destructor Documentation

6.20.2.1 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.

6.20.2.2 DakotaApproximation::DakotaApproximation (const DakotaString & *approx_type*, const ProblemDescDB & *problem_db*, const size_t & *num_acv*)

standard constructor for envelope.

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

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

copy constructor.

Copy constructor manages sharing of approxRep and incrementing of referenceCount.

6.20.2.4 DakotaApproximation::~DakotaApproximation () `[virtual]`

destructor.

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

6.20.2.5 DakotaApproximation::DakotaApproximation (BaseConstructor, const ProblemDescDB & *problem_db*, const size_t & *num_acv*) `[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 ~Dakota-Approximation).

6.20.3 Member Function Documentation

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

assignment operator.

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

6.20.3.2 DakotaApproximation * DakotaApproximation::get_approx (const DakotaString & *approx_type*, const ProblemDescDB & *problem_db*, const size_t & *num_acv*) `[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

6.21 DakotaArray Class Template Reference

Template class for the Dakota bookkeeping array.

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.

- 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!

- T & operator[ ] (int i)

  alternate bounds-checked indexing operator for int indices.

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

  alternate bounds-checked const indexing operator for int indices.

- T & operator[ ] (size_t i)

  Index operator, 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() (size_t i)

  Index operator, not bounds checked.

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

  Index operator const, not bounds checked.

- void print (ostream &s) const

  Prints a DakotaArray to an output stream.

- void read (UnPackBuffer &s)

  Reads a DakotaArray from a buffer after an MPI receive.

- void print (PackBuffer &s) const

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

- 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.

6.21.1 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 functionality needed by Dakota to the inherited base array class. The DakotaArray class can inherite from either the STL or RW vector classes.

6.21.2 Constructor & Destructor Documentation

6.21.2.1 template<class T> DakotaArray< T >::DakotaArray (const T * *p*, size_t *size*) `[inline]`

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

Assigns size values from p into array.

6.21.3 Member Function Documentation

6.21.3.1 template<class T> DakotaArray< T > & DakotaArray< T >::operator= (const T & *ival*) [inline]

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.

6.21.3.2 template<class T> DakotaArray< T >::operator T * () const [inline]

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.

6.21.3.3]

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

Index operator, returns the ith value of the array.

Index operator; calls the STL method at() which is bounds checked. Mimics the RW vector class. Note: the at() method is not supported by the __GNUC__ STL implementation and by SGI builds omitting exceptions (e.g., SIERRA).

6.21.3.4]

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

Index operator const, returns the ith value of the array.

A const version of the index operator; calls the STL method at() which is bounds checked. Mimics the RW vector class. Note: the at() method is not supported by the __GNUC__ STL implementation and by SGI builds omitting exceptions (e.g., SIERRA).

6.21.3.5 template<class T> T & DakotaArray< T >::operator() (size_t *i*) [inline]

Index operator, not bounds checked.

Non bounds check index operator, calls the STL operator[ ] which is not bounds checked. Needed to mimic the RW vector class

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

Index operator const, not bounds checked.

A const version of the non-bounds check index operator, calls the STL operator[ ] which is not bounds checked. Needed to mimic the RW vector class

6.21.3.7 template<class T> const T * DakotaArray< T >::data () const [inline]

Returns pointer T* to continuous data.

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

6.21.3.8 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.

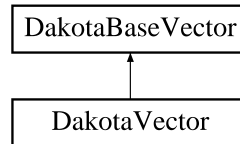
The documentation for this class was generated from the following file:

- DakotaArray.H

6.22 DakotaBaseVector Class Template Reference

Base class for the DakotaMatrix and DakotaVector classes.

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)

  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[ ] (int i)

  alternate bounds-checked indexing operator for int indices.
- const T & operator[ ] (int i) const

  alternate bounds-checked const indexing operator for int indices.
- 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).

- T & operator() (size_t i)

  Index operator, 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 const pointer to standard C array. Use with care.

Protected Methods

- T * array () const

  Returns pointer to standard C array. Use with care.

6.22.1 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

6.22.2 Constructor & Destructor Documentation

6.22.2.1 template<class T> DakotaBaseVector< T >::DakotaBaseVector (size_t *size*, const T & *initial_val*) `[inline]`

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

6.22.3 Member Function Documentation

6.22.3.1]

template<class T> T & DakotaBaseVector< T >::operator[ ] (size_t *i*) `[inline]`

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

Index operator, calls the STL method at() which is bounds checked. Mimics the RW vector class. Note: the at() method is not supported by the __GNUC__ STL implementation and by SGI builds omitting exceptions (e.g., SIERRA).

6.22.3.2]

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

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

Const versions of the index operator calls the STL method at() which is bounds checked. Mimics the RW vector class. Note: the at() method is not supported by the __GNUC__ STL implementation and by SGI builds omitting exceptions (e.g., SIERRA).

6.22.3.3 template<class T> T & DakotaBaseVector< T >::operator() (size_t *i*) `[inline]`

Index operator, not bounds checked.

Non bounds check index operator, calls the STL operator[ ] which is not bounds checked. Needed to mimic the RW vector class

6.22.3.4 template<class T> const T & DakotaBaseVector< T >::operator() (size_t *i*) const `[inline]`

Index operator const , not bounds checked.

Const version of the non-bounds check index operator, calls the STL operator[ ] which is not bounds checked. Needed to mimic the RW vector class

6.22.3.5 template<class T> size_t DakotaBaseVector< T >::length () const `[inline]`

Returns size of vector.

Returns the length of the array by calling the STL size method. Needed to mimic the RW vector class

6.22.3.6 template<class T> void DakotaBaseVector< T >::reshape (size_t *sz*) `[inline]`

Resizes vector to size sz.

Resizes the array to size sz by calling the STL resize method. Needed to mimic the RW vector class

6.22.3.7 template<class T> const T * DakotaBaseVector< T >::data () const `[inline]`

Returns const pointer to standard C array. Use with care.

Returns a const pointer to the data within the array. USE WITH CARE. Needed to mimic RW vector class.

6.22.3.8 template<class T> T * DakotaBaseVector< T >::array () const [inline, protected]

Returns pointer to standard C array. Use with care.

Returns a non-const pointer to the data within the array. Non-const version of data() used by derived classes.

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

- DakotaBaseVector.H

6.23 DakotaBiStream Class Reference

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

Public Methods

- DakotaBiStream ()

  Default constructor, need to open.

- DakotaBiStream (const char *s)

  Constructor takes name of input file.

- DakotaBiStream (const char *s, std::ios_base::openmode mode)

  Constructor takes name of input file, mode.

- DakotaBiStream (const char *s, int mode)

  Constructor takes name of input file, mode.

- ~DakotaBiStream ()

  Destructor, calls xdr_destroy to delete xdr stream.

- DakotaBiStream & operator>> (DakotaString &ds)

  Binary Input stream operator>>.

- DakotaBiStream & operator>> (char *s)

  Input operator, reads char from binary stream DakotaBiStream.*

- DakotaBiStream & operator>> (char &c)

  Input operator, reads char from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (int &i)

  Input operator, reads int from binary stream DakotaBiStream.*

- DakotaBiStream & operator>> (long &l)

  Input operator, reads long from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (short &s)

  Input operator, reads short from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (bool &b)

  Input operator, reads bool from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (double &d)

  Input operator, reads double from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (float &f)

Input operator, reads float from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (unsigned char &c)

  Input operator, reads unsigned char∗ from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (unsigned int &i)

  Input operator, reads unsigned int from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (unsigned long &l)

  Input operator, reads unsigned long from binary stream DakotaBiStream.

- DakotaBiStream & operator>> (unsigned short &s)

  Input operator, reads unsigned short from binary stream DakotaBiStream.

Private Attributes

- XDR xdrInBuf

  XDR input stream buffer.

- char inBuf [MAX_NETOBJ_SZ]

  Buffer to hold data as it is read in.

6.23.1 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. If available, the class utilize rpc/xdr to construct machine independent binary files. These Dakota restart files can be moved from host to host. The motivation to develop these classes was to replace the Rogue wave classes which Dakota historically used for binary I/O.

6.23.2 Constructor & Destructor Documentation

6.23.2.1 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.

6.23.2.2 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.

6.23.2.3 DakotaBiStream::DakotaBiStream (const char * *s*, std::ios_base::openmode *mode*)

Constructor takes name of input file, mode.

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.

6.23.2.4 DakotaBiStream::~DakotaBiStream ()

Destructor, calls xdr_destroy to delete xdr stream.

Destructor, destroys the xdr stream allocated in constructor

6.23.3 Member Function Documentation

6.23.3.1 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 DakotaString correctly.

6.23.3.2 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

6.24 DakotaBoStream Class Reference

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

Public Methods

- DakotaBoStream ()

    Default constructor, need to open.

- DakotaBoStream (const char ∗s)

    Constructor takes name of input file.

- DakotaBoStream (const char ∗s, std::ios_base::openmode mode)

    Constructor takes name of input file, mode.

- DakotaBoStream (const char ∗s, int mode)

    Constructor takes name of input file, mode.

- ∼DakotaBoStream ()

    Destructor, calls xdr_destroy to delete xdr stream.

- void testClass ()

    Performs unit testing for the DakotaBoStream class.

- DakotaBoStream & operator<< (const DakotaString &ds)

    Binary Output stream operator<<.

- DakotaBoStream & operator<< (const char ∗s)

    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 short &s)

    Output operator, writes short to binary stream DakotaBoStream.

- DakotaBoStream & operator<< (const bool &b)

    Output operator, writes bool to binary stream DakotaBoStream.

- DakotaBoStream & operator<< (const double &d)

Output operator, writes double 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 [MAX_NETOBJ_SZ]

  Buffer to hold converted data before it is written.

6.24.1 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. If available, the class utilize rpc/xdr to construct machine independent binary files. These Dakota restart files can be moved between hosts.

6.24.2 Constructor & Destructor Documentation

6.24.2.1 DakotaBoStream::DakotaBoStream ()

Default constructor, need to open.

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

6.24.2.2 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

6.24.2.3 DakotaBoStream::DakotaBoStream (const char * *s*, std::ios_base::openmode *mode*)

Constructor takes name of input file, mode.

Constructor, takes char * filename and int flags as arguments. Calls base class open method with filename and flags as arguments. Also allocates xdr stream. Note : If no rpc/xdr support xdr calls are ifdef'd out.

6.24.3 Member Function Documentation

6.24.3.1 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.

6.24.3.2 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.

6.24.3.3 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

6.25 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.

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).

- void close ()

  close graphics windows and tabular datastream.

Private Attributes

- Graphics2D ∗ graphics2D

  pointer to the 2D graphics object.

- bool win2dOn

  flag to indicate if 2D graphics window is active.

- bool 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.

- bool tabularDataFlag

  flag to indicate if tabular data stream is active.

- ofstream tabularDataFStream

  file stream for tabulation of graphics data within compute_response.

6.25.1 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).

6.25.2 Member Function Documentation

6.25.2.1 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).

6.25.2.2 void DakotaGraphics::create_tabular_datastream (const DakotaVariables & *vars*, const DakotaResponse & *response*, const DakotaString & *tabular_data_file*)

opens the tabular data file stream and prints the headings.

Opens the tabular data file stream and prints headings, one for each continuous and discrete variable and one for each response function, using the variable and response function labels. This tabular data is used for post-processing of DAKOTA results in Matlab, Tecplot, etc.

6.25.2.3 void DakotaGraphics::add_datapoint (const DakotaVariables & *vars*, const DakotaResponse & *response*)

adds data to the 2d graphics and tabular data file.

Adds data to each 2d plot and each tabular data column (one for each active variable and for each response function). graphicsCntr is used for the x axis in the graphics and the first column in the tabular data.

6.25.2.4 void DakotaGraphics::show_data_3d (DakotaRealArray & *X*, DakotaRealArray & *Y*, DakotaRealMatrix & *F*)

generate a new 3d plot for F(X,Y).

3D plotting clears data set and builds from scratch each time show_data3d is called. This still involves an event loop waiting for a mouse click (right button) to continue. X = 1-D x grid values only. Y = 1-D Y grid values only. Note that X and Y are _not_ (X,Y) pairs. F = 2-d grid of values for a single function for all (X,Y) combinations

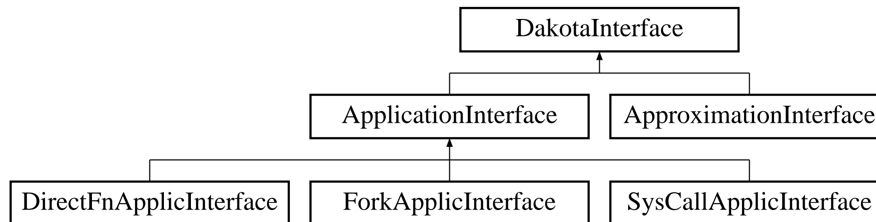
The documentation for this class was generated from the following files:

- DakotaGraphics.H
- DakotaGraphics.C

6.26 DakotaInterface Class Reference

Base class for the interface class hierarchy.

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 bool asynch_flag=0)

  the function evaluator: provides a "mapping" from the variables to the responses.

- virtual const DakotaResponseArray & synch ()

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

- virtual const DakotaResponseList & 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 void init_serial ()

  reset certain defaults for serial interface objects.

- virtual int asynch_local_evaluation_concurrency () const

  return the user-specified concurrency for asynch local evaluations.

- virtual 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, const DakotaRealVector &lower_bnds, const DakotaRealVector &upper_bnds)

  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.

- virtual const DakotaRealVectorArray & approximation_coefficients ()

  retrieve the approximation coefficients from each DakotaApproximation within an ApproximationInterface.

- void assign_rep (DakotaInterface ∗interface_rep)

  replaces existing letter with a new one.

- 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.

- bool multi_proc_eval_flag () const

  returns a flag signaling the use of multiprocessor evaluation partitions.

- bool 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 grid; 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).

- DakotaResponseArray rawResponseArray

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

- DakotaResponseList rawResponseList

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

- DakotaIntList completionList

  identifies the responses in rawResponseList for nonblocking schedules.

- bool multiProcEvalFlag

  flag for multiprocessor evaluation partitions (evalComm).

- bool iteratorDedMasterFlag

  flag for dedicated master partitioning at the iterator level.

- bool silentFlag

  flag for really quiet (silent) interface output.

- bool quietFlag

  flag for quiet interface output.

- bool verboseFlag

  flag for verbose interface output.

- bool 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.

6.26.1 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.

6.26.2 Constructor & Destructor Documentation

6.26.2.1 DakotaInterface::DakotaInterface ()

default constructor.

used in DakotaModel envelope class instantiations

6.26.2.2 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.

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

copy constructor.

Copy constructor manages sharing of interfaceRep and incrementing of referenceCount.

6.26.2.4 DakotaInterface::~DakotaInterface () `[virtual]`

destructor.

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

6.26.2.5 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).

6.26.3 Member Function Documentation

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

assignment operator.

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

6.26.3.2 void DakotaInterface::assign_rep (DakotaInterface * *interface_rep*)

replaces existing letter with a new one.

Similar to the assignment operator, the assign_rep() function decrements referenceCount for old interfaceRep, assigns the new interfaceRep, and increments referenceCount for new interfaceRep. It is different in the sense that it is used for publishing derived class letter objects, as opposed to a base class envelope object.

6.26.3.3 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.

6.26.4 Member Data Documentation

6.26.4.1 DakotaResponseArray 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.

6.26.4.2 DakotaResponseList 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. Post-processing from raw to combined form (i.e., finite difference gradient merging) is not currently supported in DakotaModel::synchronize_nowait().

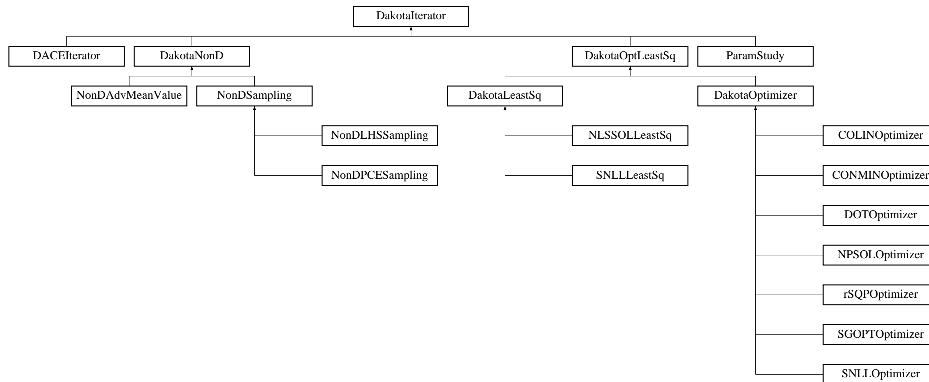
The documentation for this class was generated from the following files:

- DakotaInterface.H
- DakotaInterface.C

6.27 DakotaIterator Class Reference

Base class for the iterator class hierarchy.

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, bool all_data_flag, bool 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 DakotaVariablesArray & all_variables () const

  return the complete set of evaluated variables.

- const DakotaRealVectorArray & all_c_variables () const

  return the complete set of evaluated continuous variables.

- const DakotaResponseArray & all_responses () const

  return the complete set of computed responses.

- const DakotaRealVectorArray & all_fn_responses () const

  return the complete set of computed function responses.

- bool 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).

- virtual void update_best (const DakotaRealVector &vars, const DakotaResponse &response, const int eval_num)

compares current evaluation to best evaluation and updates best.

- void evaluate_parameter_sets (bool vars_flag, bool resp_flag, bool fns_flag, bool best_flag)

  perform function evaluations to map parameter sets (allVariables/allCVariables/allDVariables) into response sets (allResponses/allFnResponses/allGradResponses).

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.

- bool silentOutput

  flag for really quiet (silent) algorithm output.

- bool quietOutput

  flag for quiet algorithm output.

- bool verboseOutput

  flag for verbose algorithm output.

- bool debugOutput

  flag for really verbose (debug) algorithm output.

- bool asynchFlag

  copy of the model's asynchronous evaluation flag.

- DakotaVariablesArray allVariables

  array of all variables evaluated.

- DakotaRealVectorArray allCVariables

  array of all continuous variables evaluated (subset of allVariables).

- DakotaResponseArray allResponses

  array of all responses computed.

- DakotaRealVectorArray allFnResponses

  array of all function responses computed (subset of allResponses).

- DakotaStringArray allHeaders

  array of headers to insert into output while evaluating allCVariables.

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.

6.27.1 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.

6.27.2 Constructor & Destructor Documentation

6.27.2.1 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.

6.27.2.2 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.

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

copy constructor.

Copy constructor manages sharing of iteratorRep and incrementing of referenceCount.

6.27.2.4 DakotaIterator::∼DakotaIterator () [virtual]

destructor.

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

6.27.2.5 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).

6.27.2.6 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.

6.27.3 Member Function Documentation

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

assignment operator.

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

6.27.3.2 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.

6.27.3.3 void DakotaIterator::evaluate_parameter_sets (bool *vars_flag*, bool *resp_flag*, bool *fns_flag*, bool *best_flag*) [protected]

perform function evaluations to map parameter sets (allVariables/allCVariables/allDVariables) into response sets (allResponses/allFnResponses/allGradResponses).

Convenience function for derived classes with sets of function evaluations to perform (e.g., NonDSampling, DACEIterator, ParamStudy).

6.27.3.4 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.

6.27.3.5 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.

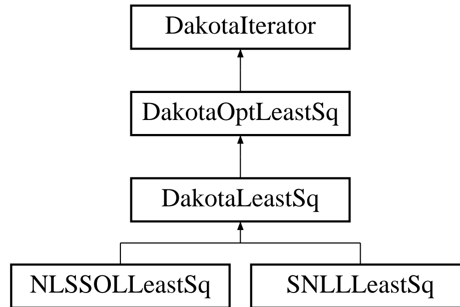
The documentation for this class was generated from the following files:

- DakotaIterator.H
- DakotaIterator.C

6.28 DakotaLeastSq Class Reference

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

Inheritance diagram for DakotaLeastSq::



Public Methods

- void run_iterator ()

  run the iterator.

- void print_iterator_results (ostream &s) const

Protected Methods

- DakotaLeastSq ()

  default constructor.

- DakotaLeastSq (DakotaModel &model)

  standard constructor.

- ~DakotaLeastSq ()

  destructor.

- virtual void minimize_residuals ()=0

  Used within the least squares branch for minimizing the sum of squares residuals. Redefines the run_iterator virtual function for the least squares branch.

Protected Attributes

- int numLeastSqTerms

  number of least squares terms.

Static Protected Attributes

- size_t staticNumLSqTerms

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

6.28.1 Detailed Description

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

The DakotaLeastSq class provides common data and functionality for NLSSOLLeastSq and SNLLLeastSq.

6.28.2 Constructor & Destructor Documentation

6.28.2.1 DakotaLeastSq::DakotaLeastSq (DakotaModel & *model*) [protected]

standard constructor.

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

6.28.3 Member Function Documentation

6.28.3.1 void DakotaLeastSq::run_iterator () [inline, 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.

6.28.3.2 void DakotaLeastSq::print_iterator_results (ostream & *s*) const [virtual]

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

Reimplemented from DakotaIterator.

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

- DakotaLeastSq.H
- DakotaLeastSq.C

6.29 DakotaList Class Template Reference

Template class for the Dakota bookkeeping list.

Public Methods

- DakotaList ()

  Default constructor.

- DakotaList (const DakotaList< T > &a)

  Copy constructor.

- ~DakotaList ()

  Destructor.

- template<class InputIter> DakotaList (InputIter first, InputIter last)

  Range constructor (member template).

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

  assignment operator.

- void testClass ()

  Class unit test method.

- void print (ostream &s) const

  Prints a DakotaList to an output stream.

- void read (UnPackBuffer &s)

  Reads a DakotaList from an UnPackBuffer after an MPI receive.

- void print (PackBuffer &s) const

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

- size_t entries () const

  Returns the number of items that are currently in the list.

- T get ()

  Removes and returns the first item in the list.

- T removeAt (size_t index)

  Removes and returns the item at the specified index.

- bool 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.

- bool contains (const T &a) const

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

- bool find (bool(∗testFun)(const T &, void ∗), void ∗d, T &k) const

  Returns TRUE if the list contains an object which the user defined function finds and sets k to this object.

- size_t index (bool(∗testFun)(const T &, void ∗), void ∗d) const

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

- void sort (bool(∗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 () const

  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).

6.29.1 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

6.29.2 Member Function Documentation

6.29.2.1 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 functionality of the class. Utilizes the assert function to test for correctness, will fail if an unexpected answer is received.

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

Removes and returns the first item in the list.

Remove and return item from front of list. Returns the object pointed to by the list::begin() iterator. It also deletes the first node by calling the list::pop_front() method. Note: get() is not the same as list::front() since the latter would return the 1st item but would not delete it.

6.29.2.3 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 the STL advance() function to step to the appropriate position in the list and then calls the list::erase() method.

6.29.2.4 template<class T> bool DakotaList< T >::remove (const T & *a*)

Removes the specified item from the list.

Removes the first instance matching object a from the list (and therefore differs from the STL list::remove() which removes all instances). Uses the STL find() algorithm to find the object and the list::erase() method to perform the remove.

6.29.2.5 template<class T> void DakotaList< T >::insert (const T & *a*) `[inline]`

Adds the item a to the end of the list.

Insert item at the end of list, calls list::push_back() method which places the object at the end of the list.

6.29.2.6 template<class T> bool DakotaList< T >::contains (const T & *a*) const `[inline]`

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

Uses the STL find() algorithm to locate the first instance of object a. Returns true if an instance is found.

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

Returns TRUE if the list contains an object which the user defined function finds and sets k to this object.

Find the first item in the list which satisfies the test function. Sets k if the object is found.

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

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

Returns the index of the first item in the list which satisfies the test function. Uses a single list traversal to both locate the object and return its index (generic algorithms would require two loop traversals).

6.29.2.9 template<class T> void DakotaList< T >::sort (bool(* *sortFun*)(const T &, const T &)) [inline]

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

The sort method utilizes the SortCompare functor and the base class list::sort algorithm to sort a list based on the incoming sorting function sortFun. Note that the functor-based sorting method of std::list is not supported by all compilers (e.g., SOLARIS, TFLOP) due to use of member templates, but a function pointer-based interface is available in some cases.

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

Returns the index of the object.

Returns the index of the first item in the list which matches the object a. Uses a single list traversal to both locate the object and return its index (generic algorithms would require two loop traversals).

6.29.2.11 template<class T> size_t DakotaList< T >::occurrencesOf (const T & *a*) const [inline]

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

Uses the STL count() algorithm to return the number of occurences of the specified object.

6.29.2.12]

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

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

Returns item at position i of the list by stepping through the list using forward or reverse STL iterators (depending on which end of the list is closer to the desired item). Once the object is found, it returns the value pointed to by the iterator.

This functionality is inefficient in 0->len loop-based list traversals and is being replaced by iterator-based list traversals in the main DAKOTA code. For isolated look-ups of a particular index, however, this approach is acceptable.

6.29.2.13]

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

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

Returns const item at position i of the list by stepping through the list using forward or reverse STL iterators (depending on which end of the list is closer to the desired item). Once the object is found it returns the value pointed to by the iterator.

This functionality is inefficient in 0->len loop-based list traversals and is being replaced by iterator-based list traversals in the main DAKOTA code. For isolated look-ups of a particular index, however, this approach is acceptable.

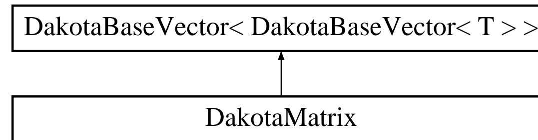
The documentation for this class was generated from the following file:

- DakotaList.H

6.30 DakotaMatrix Class Template Reference

Template class for the Dakota numerical matrix.

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.

6.30.1 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.

6.30.2 Member Function Documentation

6.30.2.1 template<class T> DakotaMatrix< T > & DakotaMatrix< T >::operator= (const T & *val*) `[inline]`

Sets all elements in the matrix to ival.

calls base class operator=(ival)

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

Class unit test method.

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

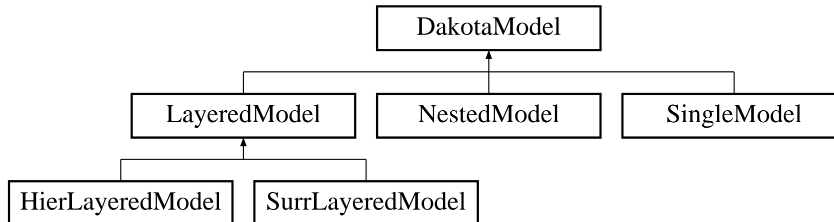
The documentation for this class was generated from the following file:

- DakotaMatrix.H

6.31 DakotaModel Class Reference

Base class for the model class hierarchy.

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 const DakotaRealVectorArray & approximation_coefficients ()

  retrieve the approximation coefficients from each DakotaApproximation within a SurrLayeredModel.

- 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 (bool correction_flag)

  manages automatic application of correction factors in LayeredModels.

- virtual void apply_correction (DakotaResponse &approx_response, const DakotaRealVector &c_-vars, bool 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 bool 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 multi-processor 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 DakotaResponseArray & synchronize ()

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

- const DakotaResponseList & 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.
- void inactive_continuous_lower_bounds (const DakotaRealVector &i_c_l_bnds)
  set the inactive continuous lower bounds in userDefinedVarConstraints.
- void inactive_continuous_upper_bounds (const DakotaRealVector &i_c_u_bnds)
  set the inactive continuous upper bounds in userDefinedVarConstraints.
- void inactive_discrete_lower_bounds (const DakotaIntVector &i_d_l_bnds)
  set the inactive discrete lower bounds in userDefinedVarConstraints.
- void inactive_discrete_upper_bounds (const DakotaIntVector &i_d_u_bnds)
  set the inactive discrete upper bounds in userDefinedVarConstraints.
- size_t num_linear_ineq_constraints () const
  return the number of linear inequality constraints.
- size_t num_linear_eq_constraints () const
  return the number of linear equality constraints.
- const 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).
- bool asynch_flag () const
  return the asynchronous evaluation flag (asynchEvalFlag).
- void asynch_flag (const bool 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.
- bool 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 DakotaResponseArray & derived_synchronize ()

  portion of synchronize() specific to derived model classes.

- virtual const DakotaResponseList & 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 DakotaResponseArray &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 bool 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. This reference is a const copy of the incoming problem_db non-const reference and is only used in DakotaModel::prob_desc_db() (it is not inherited).

- 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.

- bool asynchFDFlag

  flags use of fd_gradients w/i asynch_compute_response.

- bool asynchEvalFlag

  flags asynch evaluations (local or distributed).

- bool 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).

- bool silentFlag

  flag for really quiet (silent) model output.

- bool quietFlag

  flag for quiet model output.

- DakotaVariablesList 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.

- DakotaBoolList initialMapList

  transfers initial_map flag values from fd_gradients to synchronize_fd_gradients.

- DakotaBoolList dbFnsList

  transfers db_fns flag values from fd_gradients to synchronize_fd_gradients.

- DakotaResponseList 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.

- DakotaResponseArray 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.

- DakotaResponseList 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.

6.31.1 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.

6.31.2 Constructor & Destructor Documentation

6.31.2.1 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.

6.31.2.2 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.

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

copy constructor.

Copy constructor manages sharing of modelRep and incrementing of referenceCount.

6.31.2.4 DakotaModel::∼DakotaModel () `[virtual]`

destructor.

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

6.31.2.5 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).

6.31.3 Member Function Documentation

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

assignment operator.

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

6.31.3.2 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, ProblemDescDB's "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.

6.31.3.3 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.

6.31.3.4 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.

6.31.3.5 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.

6.31.3.6 void DakotaModel::synchronize_fd_gradients (const DakotaResponseArray & *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().

6.31.3.7 void DakotaModel::update_response (DakotaResponse & *new_response*, const DakotaIntArray & *fd_grad_asv*, const DakotaIntArray & *asv*, const bool *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.

6.31.3.8 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.

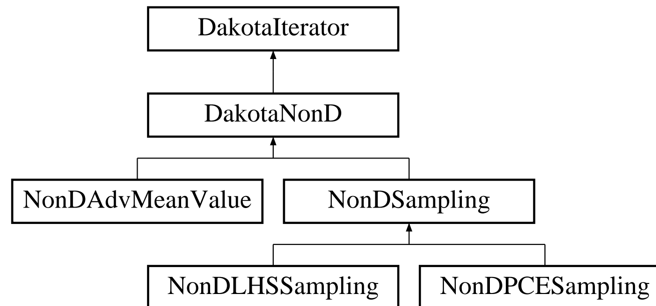
The documentation for this class was generated from the following files:

- DakotaModel.H
- DakotaModel.C

6.32 DakotaNonD Class Reference

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

Inheritance diagram for DakotaNonD::



Protected Methods

- DakotaNonD (DakotaModel &model)
  constructor.
- DakotaNonD (NoDBBaseConstructor, DakotaModel &model, int num_vars, const DakotaRealVector &lower_bnds, const DakotaRealVector &upper_bnds)
  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.
- 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.

- DakotaRealVectorArray histogramBinPairs

  histogram uncertain (x,y) bin pairs (continuous linear histogram).

- DakotaRealVectorArray histogramPointPairs

  histogram uncertain (x,y) point pairs (discrete histogram).

- 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 of response functions calculated in compute_statistics().

- DakotaRealVector mean95CIDeltas

  Plus/minus deltas on response function means for 95% confidence intervals (calculated in compute_-statistics()).

- DakotaRealVector stdDevStats

  std deviations of response functions (calculated in compute_statistics()).

- DakotaRealArray respThresh

  response thresholds for computing failure probabilities.

- DakotaRealVector probMoreThanThresh

  probabilities that response functions are greater than respThresh (calculated in compute_statistics()).

- DakotaResponse finalStatistics

  final statistics from the uncertainty propagation used in strategies: response means, standard deviations, and probabilities of failure.

- bool correlationFlag

  flag for indicating if correlation exists among the uncertain variables.

6.32.1 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.

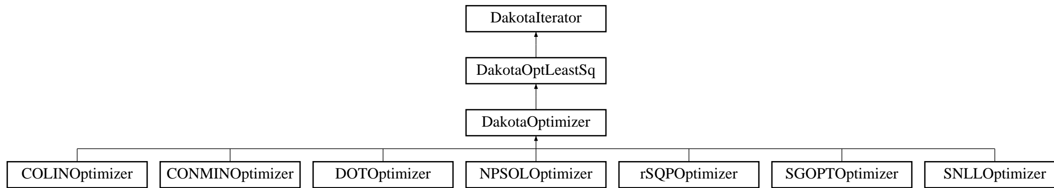
The documentation for this class was generated from the following files:

- DakotaNonD.H
- DakotaNonD.C

6.33 DakotaOptimizer Class Reference

Base class for the optimizer branch of the iterator hierarchy.

Inheritance diagram for DakotaOptimizer::



Public Methods

- void run_iterator ()

  run the iterator.

- 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 (static for use within NPSOL and OPT++ evaluator functions).

Protected Attributes

- size_t numObjectiveFunctions

  number of objective functions.

- DakotaRealVector multiObjWeights

  user-specified weights for multiple objective functions.

Static Protected Attributes

- size_t staticNumObjFns

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

- DakotaRealVector staticMultiObjWeights

  static copy of multiObjWeights for use in multi_objective_modify().

6.33.1 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.

6.33.2 Constructor & Destructor Documentation

6.33.2.1 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.

6.33.3 Member Function Documentation

6.33.3.1 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.

6.33.3.2 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.

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

maps multiple objective functions to a single objective for single-objective optimizers (static for use within NPSOL and OPT++ evaluator functions).

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.

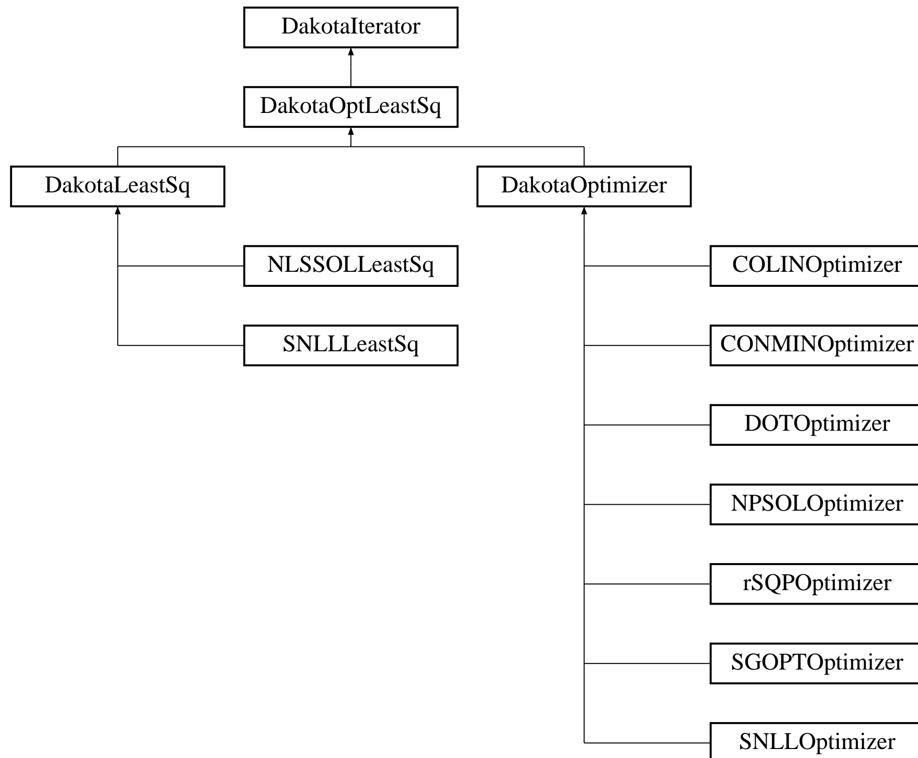
The documentation for this class was generated from the following files:

- DakotaOptimizer.H
- DakotaOptimizer.C

6.34 DakotaOptLeastSq Class Reference

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

Inheritance diagram for DakotaOptLeastSq::



Public Methods

- const DakotaVariables & iterator_variable_results () const

  return the final iterator solution (variables).

- const DakotaResponse & iterator_response_results () const

  return the final iterator solution (response).

Protected Methods

- DakotaOptLeastSq ()

  default constructor.

- DakotaOptLeastSq (DakotaModel &model)

  standard constructor.

- ~DakotaOptLeastSq ()
  destructor.

Protected Attributes

- Real convergenceTol
  optimizer/least squares convergence tolerance.
- Real constraintTol
  optimizer/least squares 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 bigRealBoundSize
  cutoff value for inequality constraint and continuous variable bounds.
- int bigIntBoundSize
  cutoff value for discrete variable 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.

- bool boundConstraintFlag

  convenience flag for denoting the presence of user-specified bound constraints. Used for method selection and error checking.

- bool speculativeFlag

  flag for speculative gradient evaluations.

- bool vendorNumericalGradFlag

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

- DakotaVariables bestVariables

  best variables found in solution.

- DakotaResponse bestResponses

  best responses found in solution.

Static Protected Attributes

- size_t staticNumContinuousVars

  static copy of numContinuousVars used in static functions passed by function pointer (NPSOL, NLSSOL, and OPT++) and in DakotaOptimizer::multi_objective_modify().

- size_t staticNumNonlinearConstraints

  static copy of numNonlinearConstraints used in static functions passed by function pointer (NPSOL, NLSSOL, and OPT++) and in DakotaOptimizer::multi_objective_modify().

6.34.1 Detailed Description

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

The DakotaOptLeastSq class provides common data and functionality for DakotaOptimizer and DakotaLeastSq.

6.34.2 Constructor & Destructor Documentation

6.34.2.1 DakotaOptLeastSq::DakotaOptLeastSq (DakotaModel & *model*) [protected]

standard constructor.

This constructor extracts inherited data for the optimizer and least squares branches and performs sanity checking on constraint settings.

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

- DakotaOptLeastSq.H
- DakotaOptLeastSq.C

6.35 DakotaResponse Class Reference

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

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.
- 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 read_tabular (istream &s)
  read responseRep::functionValues in tabular format from an istream.
- 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).

Friends

- bool operator== (const DakotaResponse &resp1, const DakotaResponse &resp2)
  equality operator.
- bool operator!= (const DakotaResponse &resp1, const DakotaResponse &resp2)
  inequality operator.

6.35.1 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.

6.35.2 Constructor & Destructor Documentation

6.35.2.1 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

6.36 DakotaResponseRep Class Reference

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

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 read_tabular (istream &s)
  read functionValues from an istream (tabular 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.

- bool operator== (const DakotaResponseRep &rep1, const DakotaResponseRep &rep2)

  equality operator.

6.36.1 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).

6.36.2 Constructor & Destructor Documentation

6.36.2.1 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.

6.36.2.2 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.

6.36.3 Member Function Documentation

6.36.3.1 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.).

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

write a responseRep object to an ostream.

ASCII version of write.

6.36.3.3 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.

6.36.3.4 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.

6.36.3.5 void DakotaResponseRep::read_tabular (istream & *s*) [private]

read functionValues from an istream (tabular format).

read_tabular is used to read functionValues in tabular format. It is currently only used by Approximation-Interfaces in reading samples from a file. There is insufficient data in a tabular file to build complete response objects; rather, the response object must be constructed a priori and then its functionValues can be set.

6.36.3.6 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.

6.36.3.7 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.

6.36.3.8 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 DakotaResponseRep::read(DakotaBoStream& s) can resize the arrays.

6.36.3.9 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.

6.36.3.10 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.

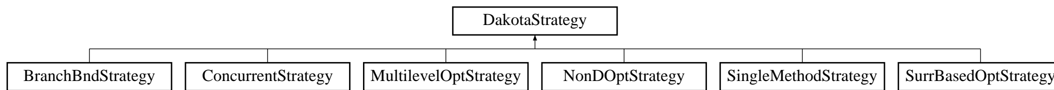
The documentation for this class was generated from the following files:

- DakotaResponse.H
- DakotaResponse.C

6.37 DakotaStrategy Class Reference

Base class for the strategy class hierarchy.

Inheritance diagram for DakotaStrategy::



Public Methods

- DakotaStrategy ()

  default constructor.

- 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.

- virtual const DakotaVariables & strategy_variable_results () const

  return the final strategy solution (variables).

- virtual const DakotaResponse & strategy_response_results () const

  return the final strategy solution (response).

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

  Convenience function for invoking an iterator and managing parallelism. This version omits communicator repartitioning. Function must be public due to use by MINLPNode.

- int world_rank () const

  return worldRank (used only 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 run_iterator_repartition (DakotaIterator &the_iterator, DakotaModel &the_model)

  Convenience function for invoking an iterator and managing parallelism. This version repartitions communicators.

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

  convenience function for allocating comms prior to running an iterator.

- void free_communicators (DakotaModel &the_model)

  convenience function for deallocating comms after running an iterator.

- 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.

- bool mpirunFlag

  flag for parallel MPI launch of DAKOTA.

- bool graphicsFlag

  flag for using graphics in a graphics executable.

- bool 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.

6.37.1 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.

6.37.2 Constructor & Destructor Documentation

6.37.2.1 DakotaStrategy::DakotaStrategy ()

default constructor.

The default constructor is used in SIERRA procedure classes. 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.

6.37.2.2 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.

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

copy constructor.

Copy constructor manages sharing of strategyRep and incrementing of referenceCount.

6.37.2.4 DakotaStrategy::∼DakotaStrategy () `[virtual]`

destructor.

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

6.37.2.5 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).

6.37.3 Member Function Documentation

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

assignment operator.

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

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

Convenience function for invoking an iterator and managing parallelism. This version omits communicator repartitioning. Function must be public due to use by MINLPNode.

This is a convenience function for encapsulating the parallel features (run/serve) of running an iterator. This function omits allocation/deallocation of communicators to provide greater efficiency in those strategies which involve multiple iterator executions but only require communicator allocation/deallocation to be performed once.

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.

6.37.3.3 void DakotaStrategy::run_iterator_repartition (DakotaIterator & *the_iterator*, DakotaModel & *the_model*) [protected]

Convenience function for invoking an iterator and managing parallelism. This version repartitions communicators.

This is a convenience function for encapsulating the parallel features (init/run/serve/free) of running an iterator. This function includes allocation/deallocation of communicators as part of each iterator invocation. Reallocating comms for each run_iterator_repartition() call can be wasteful if little is changing (e.g., BranchBndStrategy, ConcurrentStrategy). In these cases, use run_iterator() instead. This function does not require a strategyRep forward since it is only used by letter objects.

6.37.3.4 void DakotaStrategy::init_communicators (DakotaIterator & *the_iterator*, DakotaModel & *the_model*) [protected]

convenience function for allocating comms prior to running an iterator.

This is a convenience function for encapsulating the allocation of communicators prior to running an iterator. It does not require a strategyRep forward since it is only used by letter objects.

6.37.3.5 void DakotaStrategy::free_communicators (DakotaModel & *the_model*) [protected]

convenience function for deallocating comms after running an iterator.

This is a convenience function for encapsulating the deallocation of communicators after running an iterator. It does not require a strategyRep forward since it is only used by letter objects.

6.37.3.6 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 does not require a strategyRep forward since it is only used by letter objects.

6.37.3.7 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.

6.37.3.8 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

6.38 DakotaString Class Reference

DakotaString class, used as main string class for Dakota.

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.

- 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.

- 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.

- void testClass ()

  Class unit test method.

6.38.1 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

6.38.2 Member Function Documentation

6.38.2.1 DakotaString::operator const char * () const [inline]

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 Dakota-String to be used in method calls without having to call the data() or c_str() methods.

6.38.2.2 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.

6.38.2.3 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.

6.38.2.4 bool DakotaString::contains (const char * *subString*) const [inline]

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

6.38.2.5 char * DakotaString::data () const [inline]

Returns pointer to standard C char array.

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

6.38.2.6 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.

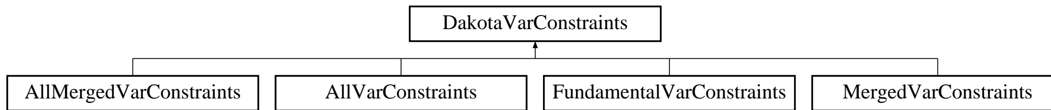
The documentation for this class was generated from the following files:

- DakotaString.H
- DakotaString.C

6.39 DakotaVarConstraints Class Reference

Base class for the variable constraints class hierarchy.

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 const DakotaRealVector & inactive_continuous_lower_bounds () const
  return the inactive continuous lower bounds.
- virtual void inactive_continuous_lower_bounds (const DakotaRealVector &i_c_l_bnds)
  set the inactive continuous lower bounds.
- virtual const DakotaRealVector & inactive_continuous_upper_bounds () const
  return the inactive continuous upper bounds.
- virtual void inactive_continuous_upper_bounds (const DakotaRealVector &i_c_u_bnds)
  set the inactive continuous upper bounds.
- virtual const DakotaIntVector & inactive_discrete_lower_bounds () const
  return the inactive discrete lower bounds.
- virtual void inactive_discrete_lower_bounds (const DakotaIntVector &i_d_l_bnds)
  set the inactive discrete lower bounds.
- virtual const DakotaIntVector & inactive_discrete_upper_bounds () const
  return the inactive discrete upper bounds.
- virtual void inactive_discrete_upper_bounds (const DakotaIntVector &i_d_u_bnds)
  set the inactive discrete upper bounds.
- virtual DakotaRealVector all_continuous_lower_bounds () const
  returns a single array with all continuous lower bounds.
- virtual DakotaRealVector all_continuous_upper_bounds () const
  returns a single array with all continuous upper bounds.
- virtual DakotaIntVector all_discrete_lower_bounds () const
  returns a single array with all discrete lower bounds.
- virtual DakotaIntVector all_discrete_upper_bounds () const
  returns a single array with all discrete 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.
- size_t num_linear_ineq_constraints () const
  return the number of linear inequality constraints.

- size_t num_linear_eq_constraints () const
  return the number of linear equality constraints.
- const 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.
- bool 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.

- DakotaRealVector emptyRealVector

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

- DakotaIntVector emptyIntVector

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

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.

6.39.1 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.

6.39.2 Constructor & Destructor Documentation

6.39.2.1 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.

6.39.2.2 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.

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

copy constructor.

Copy constructor manages sharing of varConstraintsRep and incrementing of referenceCount.

6.39.2.4 DakotaVarConstraints::∼DakotaVarConstraints () `[virtual]`

destructor.

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

6.39.2.5 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).

6.39.3 Member Function Documentation

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

assignment operator.

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

6.39.3.2 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.

6.39.3.3 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.

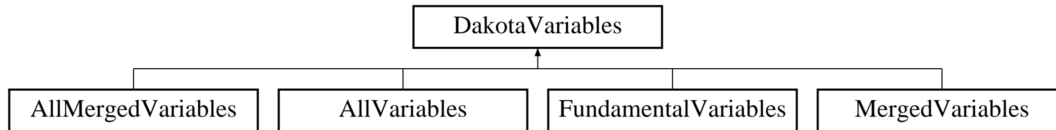
The documentation for this class was generated from the following files:

- DakotaVarConstraints.H
- DakotaVarConstraints.C

6.40 DakotaVariables Class Reference

Base class for the variables class hierarchy.

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 DakotaStringArray all_continuous_variable_labels () const
  returns a single array with all continuous variable labels.
- virtual DakotaStringArray all_discrete_variable_labels () const
  returns a single array with all discrete variable labels.
- 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.

- bool apreproFlag

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

- 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.

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

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

  equality operator.

- bool operator!= (const DakotaVariables &vars1, const DakotaVariables &vars2)

  inequality operator.

6.40.1 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.

6.40.2 Constructor & Destructor Documentation

6.40.2.1 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.

6.40.2.2 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.

6.40.2.3 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.

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

copy constructor.

Copy constructor manages sharing of variablesRep and incrementing of referenceCount.

6.40.2.5 DakotaVariables::~DakotaVariables () `[virtual]`

destructor.

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

6.40.2.6 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).

6.40.3 Member Function Documentation

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

assignment operator.

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

6.40.3.2 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).

6.40.3.3 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.

6.40.3.4 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.

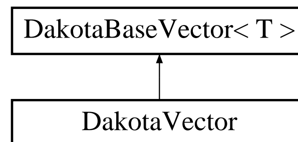
The documentation for this class was generated from the following files:

- DakotaVariables.H
- DakotaVariables.C

6.41 DakotaVector Class Template Reference

Template class for the Dakota numerical vector.

Inheritance diagram for DakotaVector::



Public Methods

- DakotaVector ()

  Default constructor.

- DakotaVector (size_t len)

  Constructor which takes an initial length.

- DakotaVector (size_t len, const T &initial_val)

  Constructor which takes an initial length and an initial value.

- DakotaVector (const DakotaVector< T > &a)

  Copy constructor.

- DakotaVector (const T *p, size_t len)

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

- ~DakotaVector ()

  Destructor.

- 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!

- 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_tabular (istream &s)

  Reads a DakotaVector from a tabular text input file.

- 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.

- void testClass ()

  Class unit test method.

6.41.1 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 DakotaBaseVector 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 functionality to read/print vectors in a variety of ways

6.41.2 Constructor & Destructor Documentation

6.41.2.1 template<class T> DakotaVector< T >::DakotaVector (const T * *p*, size_t *len*) [inline]

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

Assigns size values from p into array.

6.41.3 Member Function Documentation

6.41.3.1 template<class T> DakotaVector< T > & DakotaVector< T >::operator= (const T & *ival*) [inline]

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.

6.41.3.2 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 functionality of the class. Utilizes the assert function to test for correctness, will fail if an unexpected answer is received.

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

- DakotaVector.H

6.42 DataInterface Class Reference

Container class for interface specification data.

Public Methods

- DataInterface ()

  constructor.

- DataInterface (const DataInterface &)

  copy constructor.

- ∼DataInterface ()

  destructor.

- DataInterface & operator= (const DataInterface &)

  assignment operator.

- bool operator== (const DataInterface &)

  equality operator.

- void write (ostream &s) const

  write a DataInterface object to an ostream.

- void read (UnPackBuffer &s)

  read a DataInterface object from a packed MPI buffer.

- void write (PackBuffer &s) const

  write a DataInterface object to a packed MPI buffer.

Public Attributes

- DakotaString interfaceType

  the interface selection: application_system/fork/direct/grid 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***).*

- bool apreproFormatFlag

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

- bool fileTagFlag

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

- bool 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***).*

- DakotaString modelCenterFile

  configuration file for defining the simulation model accessed via the direct interface to the ModelCenter framework from Phoenix Integration (from the `modelcenter_file` *specification in* **InterfApplic***).*

- DakotaStringList gridHostNames

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

- DakotaIntArray gridProcsPerHost

  processors per host machine for a grid 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***).*

- bool activeSetVectorFlag

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

- bool evalCacheFlag

  function evaluation cache: 1=active (all new evaluations checked against existing cache and then added to cache), 0=inactive (cache neither queried nor augmented) (from the `deactivate evaluation_cache` *specification in* **InterfApplic***).*

- bool restartFileFlag

  function evaluation cache: 1=active (all new evaluations written to restart), 0=inactive (no records written to restart) (from the `deactivate restart_file` *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, region, or file (from the `reuse_samples` *specification in* **InterfApprox***).*

- DakotaString approxSampleReuseFile

  the file name for the "file" setting for the `reuse_samples` *specification in* **InterfApprox***.*

- DakotaString approxCorrectionType

  correction type for global and hierarchical approximations: additive or multiplicative (from the `correction` *specification in* **InterfApprox***).*

- DakotaString approxCorrectionOrder

  correction order for global and hierarchical approximations: zeroth or first (from the `correction` *specification in* **InterfApprox***).*

- bool 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***).*

- int polynomialOrder

  scalar integer indicating the order of the polynomial approximation (1=linear, 2=quadratic, 3=cubic).

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).

6.42.1 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

6.43 DataMethod Class Reference

Container class for method specification data.

Public Methods

- DataMethod ()

  constructor.

- DataMethod (const DataMethod &)

  copy constructor.

- ~DataMethod ()

  destructor.

- DataMethod & operator= (const DataMethod &)

  assignment operator.

- bool operator== (const DataMethod &)

  equality operator.

- void write (ostream &s) const

  write a DataMethod object to an ostream.

- void read (UnPackBuffer &s)

  read a DataMethod object from a packed MPI buffer.

- void write (PackBuffer &s) const

  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***).*

- bool speculativeFlag

  flag for use of speculative gradient approaches for maintaining parallel load balance during the line search portion of optimization algorithms (from the `speculative` *specification in* **MethodIndControl***).*

- 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 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 nonlinear interior-point 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 nonlinear interior-point methods in* **MethodOPTPPDC**.

- DakotaString centralPath

  the `central_path` *specification for nonlinear interior-point methods in* **MethodOPTPPDC**.

- Real stepLenToBoundary

the steplength_to_boundary *specification for nonlinear interior-point methods in* **MethodOPTPPDC**.

- Real centeringParam

  the centering_parameter *specification for nonlinear interior-point methods in* **MethodOPTPPDC**.

- int searchSchemeSize

  the search_scheme_size *specification for PDS methods in* **MethodOPTPPDC**.

- Real 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**.

- bool nonAdaptiveFlag

  the non_adaptive *specification for the pga_real method in* **MethodSGOPTEA**.

- bool randomizeOrderFlag

  the stochastic *specification for the PS method in* **MethodSGOPTPS**.

- bool 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**.

- DakotaString daceMethod

  the dace method selection: grid, random, oas, lhs, oa_lhs, box_behnken, or central_composite (from the `dace` *specification in* **MethodDACE**).

- int numSymbols

  the `symbols` *specification for DACE methods.*

- int randomSeed

  the `seed` *specification for SGOPT, NonD, & DACE methods.*

- int numSamples

  the `samples` *specification for NonD & DACE methods.*

- bool fixedSeedFlag

  flag for fixing the value of the seed among different NonD/DACE sample sets. This results in the use of the same sampling stencil/pattern throughout a strategy with repeated sampling.

- 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**.

- bool 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).

6.43.1 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

6.44 DataResponses Class Reference

Container class for responses specification data.

Public Methods

- DataResponses ()

  constructor.

- DataResponses (const DataResponses &)

  copy constructor.

- ~DataResponses ()

  destructor.

- DataResponses & operator= (const DataResponses &)

  assignment operator.

- bool operator== (const DataResponses &)

  equality operator.

- void write (ostream &s) const

  write a DataResponses object to an ostream.

- void read (UnPackBuffer &s)

  read a DataResponses object from a packed MPI buffer.

- void write (PackBuffer &s) const

  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 numLeastSqTerms

  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***).*

- DakotaStringArray responseLabels

  the response labels array (from the `response_descriptors` *specification in* **RespLabels***).*

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).

6.44.1 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

6.45 DataStrategy Class Reference

Container class for strategy specification data.

Public Methods

- DataStrategy ()

  constructor.

- DataStrategy (const DataStrategy &)

  copy constructor.

- ~DataStrategy ()

  destructor.

- DataStrategy & operator= (const DataStrategy &)

  assignment operator.

- void write (ostream &s) const

  write a DataStrategy object to an ostream.

- void read (UnPackBuffer &s)

  read a DataStrategy object from a packed MPI buffer.

- void write (PackBuffer &s) const

  write a DataStrategy object to a packed MPI buffer.

Public Attributes

- DakotaString strategyType

  the strategy selection: multi_level, surrogate_based_opt, opt_under_uncertainty, branch_and_bound, multi_-start, pareto_set, or single_method.

- bool graphicsFlag

  flags use of graphics by the strategy (from the graphics specification in **StratIndControl***).*

- bool tabularDataFlag

  flags tabular data collection by the strategy (from the tabular_graphics_data specification in **StratInd-Control***).*

- DakotaString tabularDataFile

  the filename used for tabular data collection by the strategy (from the tabular_graphics_file specification in **StratIndControl***).*

- int iteratorServers

number of servers for concurrent iterator parallelism (from the iterator_servers specification in **StratIndControl***).*

- DakotaString iteratorScheduling

  type of scheduling (self or static) used in concurrent iterator parallelism (from the iterator_self_scheduling and iterator_static_scheduling specifications in **StratIndControl***).*

- DakotaString methodPointer

  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 branchBndNumSamplesRoot

  number of samples at the root for the branch and bound strategy (from the num_samples_at_root specification in **StratBandB***).*

- int branchBndNumSamplesNode

  number of samples at each node for the branch and bound strategy (from the num_samples_at_node specification in **StratBandB***).*

- DakotaStringList multilevelMethodList

  list of methods for the multilevel hybrid optimization strategy (from the method_list specification in **StratML***).*

- DakotaString multilevelType

  the type of multilevel hybrid optimization strategy: uncoupled, uncoupled_adaptive, or coupled (from the uncoupled, adaptive, and coupled specifications in **StratML***).*

- Real multilevelProgThresh

  progress threshold for uncoupled_adaptive multilevel hybrids (from the progress_threshold specification in **StratML***).*

- DakotaString multilevelGlobalMethodPointer

  global method pointer for coupled multilevel hybrids (from the global_method_pointer specification in **StratML***).*

- DakotaString multilevelLocalMethodPointer

  local method pointer for coupled multilevel hybrids (from the local_method_pointer specification in **StratML***).*

- Real multilevelLSProb

  local search probability for coupled multilevel hybrids (from the local_search_probability specification in **StratML***).*

- int surrBasedOptMaxIterations

  maximum number of iterations in the surrogate-based optimization strategy (from the max_iterations specification in **StratSBO***).*

- Real surrBasedOptConvTol

  convergence tolerance in the surrogate-based optimization strategy (from the convergence_tolerance specification in **StratSBO***).*

- int surrBasedOptSoftConvLimit

number of consecutive iterations with change less than surrBasedOptConvTol required to trigger convergence within the surrogate-based optimization strategy (from the soft_convergence_limit specification in **StratSBO***).*

- Real surrBasedOptTRInitSize

  initial trust region size in the surrogate-based optimization strategy (from the initial_size specification in **StratSBO***) note: this is a relative value, e.g., 0.1 = 10% of global bounds distance (upper bound - lower bound) for each variable.*

- Real surrBasedOptTRMinSize

  minimum trust region size in the surrogate-based optimization strategy (from the minimum_size specification in **StratSBO***), if the trust region size falls below this threshold the SBO iterations are terminated (note: if kriging is used with SBO, the min trust region size is set to 1.0e-3 in attempt to avoid ill-conditioned matrixes that arise in kriging over small trust).*

- Real surrBasedOptTRContractTrigger

  trust region minimum improvement level (ratio of actual to predicted decrease in objective fcn) in the surrogate-based optimization strategy (from the contract_region_threshold specification in **StratSBO***), the trust region shrinks or is rejected if the ratio is below this value ("eta_1" in the Conn-Gould-Toint trust region book.*

- Real surrBasedOptTRExpandTrigger

  trust region sufficient improvement level (ratio of actual to predicted decrease in objective fcn) in the surrogate-based optimization strategy (from the expand_region_threshold specification in **StratSBO***), the trust region expands if the ratio is above this value ("eta_2" in the Conn-Gould-Toint trust region book).*

- Real surrBasedOptTRContract

  trust region contraction factor in the surrogate-based optimization strategy (from the contraction_factor specification in **StratSBO***).*

- Real surrBasedOptTRExpand

  trust region expansion factor in the surrogate-based optimization strategy (from the expansion_factor specification in **StratSBO***).*

- int concurrentRandomJobs

  number of random jobs to perform in the concurrent strategy (from the random_starts and random_weight_-sets specifications in **StratMultiStart** *and* **StratParetoSet***).*

- int concurrentSeed

  seed for the selected random jobs within the concurrent strategy (from the seed specification in **StratMultiStart** *and* **StratParetoSet***).*

- DakotaRealVector concurrentParameterSets

  user-specified (i.e., nonrandom) parameter sets to evaluate in the concurrent strategy (from the starting_-points and multi_objective_weight_sets specifications in **StratMultiStart** *and* **StratParetoSet***).*

Private Methods

- void assign (const DataStrategy &data_strategy)

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

6.45.1 Detailed Description

Container class for strategy specification data.

The DataStrategy class is used to contain the data from a strategy keyword specification. It is populated by ProblemDescDB::strategy_kwhandler() and is queried by the ProblemDescDB::get_<datatype>() functions. Default values are managed in the DataStrategy constructor. Data is public to avoid maintaining set/get functions, but is still encapsulated within ProblemDescDB since ProblemDescDB::strategySpec 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:

- DataStrategy.H
- DataStrategy.C

6.46 DataVariables Class Reference

Container class for variables specification data.

Public Methods

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

- 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_descriptors` *specification in* **VarDV***).*

- DakotaStringArray discreteDesignLabels

  the discrete design labels array (from the `ddv_descriptors` *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***).*

- DakotaRealVectorArray histogramUncBinPairs

  an array containing a vector of (x,y) pairs for each bin-based histogram uncertain variable (see continuous linear histogram in LHS manual; from the `huv_num_bin_pairs` *and* `huv_bin_pairs` *specifications in* **VarUV***).*

- DakotaRealVectorArray histogramUncPointPairs

  an array containing a vector of (x,y) pairs for each point-based histogram uncertain variable (see discrete histogram in LHS manual; from the `huv_num_point_pairs` *and* `huv_point_pairs` *specifications 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_descriptors`, `lnuv_descriptors`, `uuv_descriptors`, `luuv_descriptors`, `wuv_descriptors`, *and* `huv_descriptors` *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_descriptors` *specification in* **VarSV***).*

- DakotaStringArray discreteStateLabels

  the discrete state labels array (from the `dsv_descriptors` *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).

6.46.1 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).

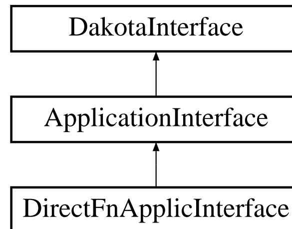
The documentation for this class was generated from the following files:

- DataVariables.H
- DataVariables.C

6.47 DirectFnApplicInterface Class Reference

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

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 (DakotaPRPList &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 (DakotaPRPList &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().

Protected 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.

Protected Attributes

- DakotaString iFilterName

  name of the direct function input filter.

- DakotaString oFilterName

  name of the direct function output filter.

- DakotaString pxcFile

  name of the ModelCenter simulation config file.

- bool gradFlag

  signals use of fnGrads in direct simulator functions.

- bool hessFlag

  signals use of fnHessians in direct simulator functions.

- size_t numFns

  number of functions in fnVals.

- size_t numVars

  total number of continuous and discrete variables.

- size_t 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.

Private Methods

- int cantilever (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  the cantilever optimization under uncertainty test function.

- 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 text_book_ouu (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  the text_book_ouu optimization under uncertainty test function.

- int salinas (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  direct interface to the SALINAS structural dynamics simulation code.

- int mc_api_run (const DakotaVariables &vars, const DakotaIntArray &asv, DakotaResponse &response)

  Call ModelCenter via API, HKIM 4/3/03.

6.47.1 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.

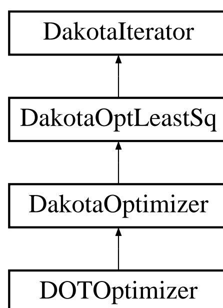
The documentation for this class was generated from the following files:

- DirectFnApplicInterface.H
- DirectFnApplicInterface.C

6.48 DOTOptimizer Class Reference

Wrapper class for the DOT optimization library.

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.

- int realWorkSpaceSize

  size of realWorkSpace.

- int intWorkSpaceSize

  size of intWorkSpace.

- DakotaRealArray realWorkSpace

  real work space for DOT.

- DakotaIntArray intWorkSpace

  int work space for 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.

6.48.1 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.

6.48.2 Member Data Documentation

6.48.2.1 int DOTOptimizer::dotInfo [private]

INFO from DOT manual.

Information requested by DOT: 0=optimization complete, 1=get values, 2=get gradients

6.48.2.2 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).

6.48.2.3 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.

6.48.2.4 int DOTOptimizer::printControl [private]

IPRINT from DOT manual (controls output verbosity).

Values range from 0 (least output) to 7 (most output).

6.48.2.5 int DOTOptimizer::optimizationType [private]

MINMAX from DOT manual (minimize or maximize).

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

6.48.2.6 DakotaRealArray DOTOptimizer::realCntlParmArray [private]

RPRM from DOT manual.

Array of real control parameters.

6.48.2.7 DakotaIntArray DOTOptimizer::intCntlParmArray [private]

IPRM from DOT manual.

Array of integer control parameters.

6.48.2.8 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).

6.48.2.9 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.

6.48.2.10 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.

6.48.2.11 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

6.49 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.

6.49.1 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.

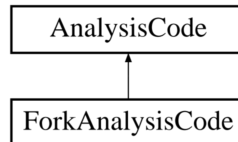
The documentation for this struct was generated from the following file:

- CtelRegExp.C

6.50 ForkAnalysisCode Class Reference

Derived class in the AnalysisCode class hierarchy which spawns simulations using forks.

Inheritance diagram for ForkAnalysisCode::



Public Methods

- ForkAnalysisCode (const ProblemDescDB &problem_db)

  constructor.

- ~ForkAnalysisCode ()

  destructor.

- pid_t fork_program (const bool 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).*

6.50.1 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.

6.50.2 Member Function Documentation

6.50.2.1 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().

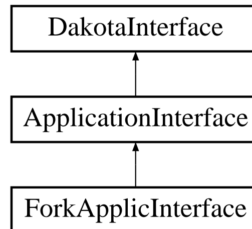
The documentation for this class was generated from the following files:

- ForkAnalysisCode.H
- ForkAnalysisCode.C

6.51 ForkApplicInterface Class Reference

Derived application interface class which spawns simulation codes using forks.

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 (DakotaPRPList &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 (DakotaPRPList &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 (DakotaPRPList &prp_list, const pid_t pid)

  Convenience function for common code between derived_synch() & derived_synch_nowait().

- pid_t fork_application (const bool 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.

6.51.1 Detailed Description

Derived application interface class which spawns simulation codes using forks.

ForkApplicInterface uses a ForkAnalysisCode object for performing simulation invocations.

6.51.2 Member Function Documentation

6.51.2.1 pid_t ForkApplicInterface::fork_application (const bool *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.

6.51.2.2 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.

6.51.2.3 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().

6.51.2.4 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

6.52 FunctionCompare Class Template Reference

Public Methods

- FunctionCompare (bool(*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

- bool(* testFunction)(const T &, void *)

  Pointer to test function.

- void * search_val

  Holds the value to search for.

6.52.1 Detailed Description

template<class T> class FunctionCompare< T >

Internal functor to mimic 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.

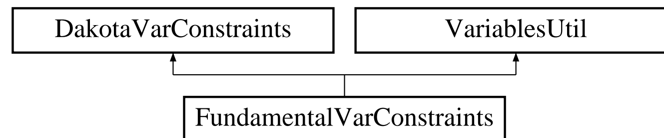
The documentation for this class was generated from the following file:

- DakotaList.H

6.53 FundamentalVarConstraints Class Reference

Derived class within the DakotaVarConstraints hierarchy which employs the default data view (no variable or domain type array merging).

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.

- const DakotaRealVector & inactive_continuous_lower_bounds () const

return the inactive continuous lower bounds.

- void inactive_continuous_lower_bounds (const DakotaRealVector &i_c_l_bnds)

  set the inactive continuous lower bounds.

- const DakotaRealVector & inactive_continuous_upper_bounds () const

  return the inactive continuous upper bounds.

- void inactive_continuous_upper_bounds (const DakotaRealVector &i_c_u_bnds)

  set the inactive continuous upper bounds.

- const DakotaIntVector & inactive_discrete_lower_bounds () const

  return the inactive discrete lower bounds.

- void inactive_discrete_lower_bounds (const DakotaIntVector &i_d_l_bnds)

  set the inactive discrete lower bounds.

- const DakotaIntVector & inactive_discrete_upper_bounds () const

  return the inactive discrete upper bounds.

- void inactive_discrete_upper_bounds (const DakotaIntVector &i_d_u_bnds)

  set the inactive discrete upper bounds.

- DakotaRealVector all_continuous_lower_bounds () const

  returns a single array with all continuous lower bounds.

- DakotaRealVector all_continuous_upper_bounds () const

  returns a single array with all continuous upper bounds.

- DakotaIntVector all_discrete_lower_bounds () const

  returns a single array with all discrete lower bounds.

- DakotaIntVector all_discrete_upper_bounds () const

  returns a single array with all discrete 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

- bool 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.

6.53.1 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).

6.53.2 Constructor & Destructor Documentation

6.53.2.1 FundamentalVarConstraints::FundamentalVarConstraints (const ProblemDescDB & *problem_db*)

constructor.

Extract fundamental lower and upper bounds (VariablesUtil is not used).

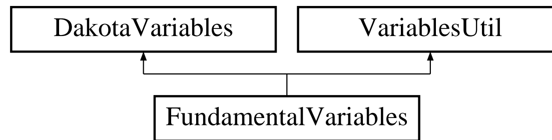
The documentation for this class was generated from the following files:

- FundamentalVarConstraints.H
- FundamentalVarConstraints.C

6.54 FundamentalVariables Class Reference

Derived class within the DakotaVariables hierarchy which employs the default data view (no variable or domain type array merging).

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.

- DakotaStringArray all_continuous_variable_labels () const

  returns a single array with all continuous variable labels.

- DakotaStringArray all_discrete_variable_labels () const

  returns a single array with all discrete variable labels.

- 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

- bool 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.

Friends

- bool operator== (const FundamentalVariables &vars1, const FundamentalVariables &vars2)

  equality operator.

6.54.1 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)).

6.54.2 Constructor & Destructor Documentation

6.54.2.1 FundamentalVariables::FundamentalVariables (const ProblemDescDB & *problem_db*)

standard constructor.

Extract fundamental variable types and labels (VariablesUtil is not used).

6.54.3 Friends And Related Function Documentation

6.54.3.1 bool operator== (const FundamentalVariables & *vars1*, const FundamentalVariables & *vars2*) `[friend]`

equality operator.

Check each fundamental array using operator== from data_types.C. Labels are ignored.

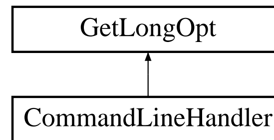
The documentation for this class was generated from the following files:

- FundamentalVariables.H
- FundamentalVariables.C

6.55 GetLongOpt Class Reference

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

Inheritance diagram for GetLongOpt::



Public Types

- enum OptType { **Valueless**, **OptionalValue**, **MandatoryValue** }

  enum for different types of values associated with command line options.

Public 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.

6.55.1 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 "=".

6.55.2 Constructor & Destructor Documentation

6.55.2.1 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.

6.55.3 Member Function Documentation

6.55.3.1 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.

6.55.3.2 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.

6.55.3.3 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.

6.55.3.4 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.

6.55.3.5 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.

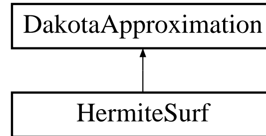
The documentation for this class was generated from the following files:

- CommandLineHandler.H
- CommandLineHandler.C

6.56 HermiteSurf Class Reference

Derived approximation class for Hermite polynomials (global approximation).

Inheritance diagram for HermiteSurf::



Public Methods

- HermiteSurf (const ProblemDescDB &problem_db, const size_t &num_acv)

  constructor.

- ~HermiteSurf ()

  destructor.

Protected Methods

- int required_samples ()

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

- const DakotaRealVector & approximation_coefficients ()

  return the coefficient array computed by find_coefficients().

- void find_coefficients ()

  find the Polynomial Chaos coefficients for the response surface.

- Real get_value (const DakotaRealVector &x)

  retrieve the function value for a given parameter set x.

Private Methods

- void get_num_chaos ()

  calculate number of Chaos according to the highest order of Chaos.

- 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.

6.56.1 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).

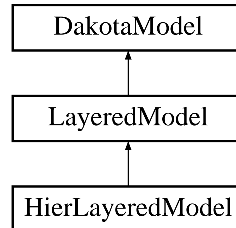
The documentation for this class was generated from the following files:

- HermiteSurf.H
- HermiteSurf.C

6.57 HierLayeredModel Class Reference

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

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 DakotaResponseArray & derived_synchronize ()

  portion of synchronize() specific to HierLayeredModel.

- const DakotaResponseList & 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 lowFidelity-Interface).

- bool derived_master_overload () const

  flag which prevents overloading the master with a multiprocessor evaluation (request forwarded to low-FidelityInterface).

- 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.

6.57.1 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.

6.57.2 Member Function Documentation

6.57.2.1 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.

6.57.2.2 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.

6.57.2.3 const DakotaResponseArray & 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.

6.57.2.4 const DakotaResponseList & 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

6.58 KrigApprox Class Reference

Utility class for kriging interpolation.

Public Methods

- KrigApprox (int, int, const DakotaRealVector &, const DakotaRealVector &, const DakotaRealVector &)

  constructor.

- ~KrigApprox ()

  destructor.

- void ModelBuild (int, int, const DakotaRealVector &, const DakotaRealVector &, bool)

  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 * conminThetaVars

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

- Real * conminThetaLowerBnds

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

- Real * conminThetaUpperBnds

  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.

6.58.1 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.

6.58.2 Member Function Documentation

6.58.2.1 Real KrigApprox::ModelApply (int, int, const DakotaRealVector &)

Function returns a response value using the kriging surface.

The response value is computed at the design point specified by the DakotaRealVector function argument.

6.58.3 Member Data Documentation

6.58.3.1 int KrigApprox::N1 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

N1 = number of variables + 2

6.58.3.2 int KrigApprox::N2 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

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

6.58.3.3 int KrigApprox::N3 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

N3 = Maximum possible number of active constraints.

6.58.3.4 int KrigApprox::N4 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

N4 = Maximum(N3,number of variables)

6.58.3.5 int KrigApprox::N5 `[private]`

Size variable for CONMIN arrays. See CONMIN manual.

N5 = 2∗(N4)

6.58.3.6 Real KrigApprox::CT `[private]`

CONMIN variable: Constraint thickness parameter.

The value of CT decreases in magnitude during optimization.

6.58.3.7 Real* KrigApprox::S [private]

Internal CONMIN array.

Move direction in N-dimensional space.

6.58.3.8 Real* KrigApprox::G1 [private]

Internal CONMIN array.

Temporary storage of constraint values.

6.58.3.9 Real* KrigApprox::G2 [private]

Internal CONMIN array.

Temporary storage of constraint values.

6.58.3.10 Real* KrigApprox::B [private]

Internal CONMIN array.

Temporary storage for computations involving array S.

6.58.3.11 Real* KrigApprox::C [private]

Internal CONMIN array.

Temporary storage for use with arrays B and S.

6.58.3.12 int* KrigApprox::MS1 [private]

Internal CONMIN array.

Temporary storage for use with arrays B and S.

6.58.3.13 Real* KrigApprox::SCAL [private]

Internal CONMIN array.

Vector of scaling parameters for design parameter values.

6.58.3.14 Real* KrigApprox::DF [private]

Internal CONMIN array.

Temporary storage for analytic gradient data.

6.58.3.15 Real* KrigApprox::A [private]

Internal CONMIN array.

Temporary 2-D array for storage of constraint gradients.

6.58.3.16 int* KrigApprox::ISC [private]

Internal CONMIN array.

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

6.58.3.17 int* KrigApprox::IC [private]

Internal CONMIN array.

Array of flags to identify active and violated constraints

6.58.3.18 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.

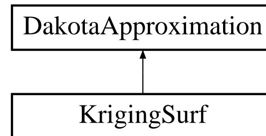
The documentation for this class was generated from the following files:

- KSMSurf.H
- KSMSurf.C

6.59 KrigingSurf Class Reference

Derived approximation class for kriging interpolation.

Inheritance diagram for KrigingSurf::



Public Methods

- KrigingSurf (const ProblemDescDB &problem_db, const size_t &num_acv)

  constructor.

- ~KrigingSurf ()

  destructor.

Protected Methods

- void find_coefficients ()

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

- int required_samples ()

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

- bool runConminFlag

  Flag to run CONMIN (value=1) or use user-supplied correlations (value=0).

6.59.1 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.

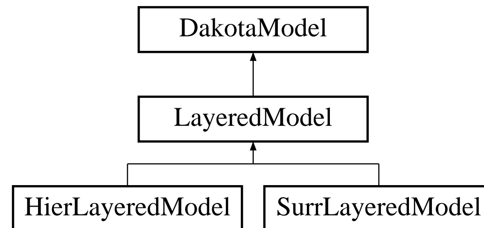
The documentation for this class was generated from the following files:

- KSMSurf.H
- KSMSurf.C

6.60 LayeredModel Class Reference

Base class for the layered models (SurrLayeredModel and HierLayeredModel).

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, bool 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).

- bool force_rebuild ()

  evaluate whether a rebuild of the approximation should be forced based on changes in the inactive data.

- void auto_correction (bool correction_flag)

  sets autoCorrection to ON (1) or OFF (0).

Protected Attributes

- DakotaResponseArray correctedResponseArray

  array of corrected responses used in derived_synchronize() functions.

- DakotaResponseList correctedResponseList

  list of corrected responses used in derived_synchronize_nowait() functions.

- DakotaRealVectorList 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

  approximation correction approach to be used: additive or multiplicative.

- DakotaString correctionOrder

  approximation correction order to be used: zeroth or first.

- int approxBuilds

  number of calls to build_approximation().

- bool autoCorrection

  a flag which controls the use of apply_correction() in SurrLayeredModel and HierLayeredModel approximate response computations.

- DakotaString approxType

  approximation type identifier string: global, local, or hierarchical.

- DakotaString refitInactive

  flag denoting a user setting for rebuilding the approximation when changes occur to the inactive variables data.

- DakotaRealVector fitInactiveCVars

  stores a copy of the inactive continuous variables when the approximation is built; used to detect when a rebuild is required.

- DakotaRealVector fitInactiveCLowerBnds

  stores a copy of the inactive continuous lower bounds when the approximation is built; used to detect when a rebuild is required.

- DakotaRealVector fitInactiveCUpperBnds

  stores a copy of the inactive continuous upper bounds when the approximation is built; used to detect when a rebuild is required.

- DakotaIntVector fitInactiveDVars

  stores a copy of the inactive discrete variables when the approximation is built; used to detect when a rebuild is required.

- DakotaIntVector fitInactiveDLowerBnds

  stores a copy of the inactive discrete lower bounds when the approximation is built; used to detect when a rebuild is required.

- DakotaIntVector fitInactiveDUpperBnds

  stores a copy of the inactive discrete upper bounds when the approximation is built; used to detect when a rebuild is required.

Private Attributes

- DakotaRealVector offsetValues

  values used to offset the function values in an approximate response in order to apply a truth model correction.

- DakotaRealVector scaleFactors

  values used to scale the function values, gradients, and Hessians in an approximate response in order to apply a truth model correction.

- bool correctionComputed

  flag used to indicate whether or not a correction is available.

- bool badScalingFlag

  flag used to indicate function values near zero for multiplicative corrections; triggers an automatic switch to additive corrections.

- DakotaRealVector betaFns

  1st-order correction term: If multiplicative (beta), then equals the ratio of high fidelity to low fidelity model values at x=x_center. If additive, then equals the difference between high and low fidelity model values at x=x_center.

- DakotaRealMatrix betaGrads

  1st-order correction term: If multiplicative (beta), then equals the gradient of the high/low function ratio at x=x_center. If additive, then equals the gradient of the high/low function difference at x=x_center.

- DakotaRealVector betaCenterPt

  1st-order correction 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.

6.60.1 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.

6.60.2 Member Function Documentation

6.60.2.1 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.

6.60.2.2 bool LayeredModel::force_rebuild () [protected]

evaluate whether a rebuild of the approximation should be forced based on changes in the inactive data.

This function forces a rebuild of the approximation according to the approximation type, the refitInactive setting, and whether any inactive data has changed since the last build.

6.60.3 Member Data Documentation

6.60.3.1 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().

6.60.3.2 bool 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.

6.60.3.3 DakotaString LayeredModel::refitInactive [protected]

flag denoting a user setting for rebuilding the approximation when changes occur to the inactive variables data.

A setting of "all" denotes that the approximation should be rebuilt every time the inactive variables change (e.g., for each instance of {d} in OUU). A setting of "region" denotes that the approximation should be rebuilt every time the bounded region for the inactive variables changes (e.g., for each new trust region on {d} in OUU).

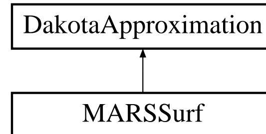
The documentation for this class was generated from the following files:

- LayeredModel.H
- LayeredModel.C

6.61 MARSSurf Class Reference

Derived approximation class for multivariate adaptive regression splines.

Inheritance diagram for MARSSurf::



Public Methods

- MARSSurf (const ProblemDescDB &problem_db, const size_t &num_acv)

    constructor.

- ~MARSSurf ()

    destructor.

Protected Methods

- int required_samples ()

    return the minimum number of samples required to build the derived class approximation type in numVars 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).

6.61.1 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.

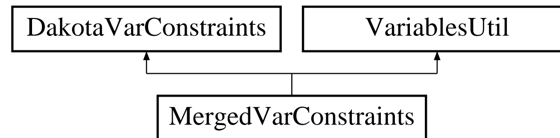
The documentation for this class was generated from the following files:

- MARSSurf.H
- MARSSurf.C

6.62 MergedVarConstraints Class Reference

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

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.

- const DakotaRealVector & inactive_continuous_lower_bounds () const

  return the inactive continuous lower bounds.

- void inactive_continuous_lower_bounds (const DakotaRealVector &i_c_l_bnds)
  set the inactive continuous lower bounds.
- const DakotaRealVector & inactive_continuous_upper_bounds () const
  return the inactive continuous upper bounds.
- void inactive_continuous_upper_bounds (const DakotaRealVector &i_c_u_bnds)
  set the inactive continuous upper bounds.
- const DakotaIntVector & inactive_discrete_lower_bounds () const
  return the inactive discrete lower bounds.
- void inactive_discrete_lower_bounds (const DakotaIntVector &i_d_l_bnds)
  set the inactive discrete lower bounds.
- const DakotaIntVector & inactive_discrete_upper_bounds () const
  return the inactive discrete upper bounds.
- void inactive_discrete_upper_bounds (const DakotaIntVector &i_d_u_bnds)
  set the inactive discrete upper bounds.
- DakotaRealVector all_continuous_lower_bounds () const
  returns a single array with all continuous lower bounds.
- DakotaRealVector all_continuous_upper_bounds () const
  returns a single array with all continuous upper bounds.
- DakotaIntVector all_discrete_lower_bounds () const
  returns a single array with all discrete lower bounds.
- DakotaIntVector all_discrete_upper_bounds () const
  returns a single array with all discrete 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).

6.62.1 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).

6.62.2 Constructor & Destructor Documentation

6.62.2.1 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).

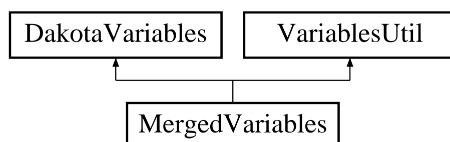
The documentation for this class was generated from the following files:

- MergedVarConstraints.H
- MergedVarConstraints.C

6.63 MergedVariables Class Reference

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

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.
- DakotaStringArray all_continuous_variable_labels () const
  returns a single array with all continuous variable labels.
- DakotaStringArray all_discrete_variable_labels () const
  returns a single array with all discrete variable labels.
- 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.

Friends

- bool operator== (const MergedVariables &vars1, const MergedVariables &vars2)

  equality operator.

6.63.1 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)).

6.63.2 Constructor & Destructor Documentation

6.63.2.1 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).

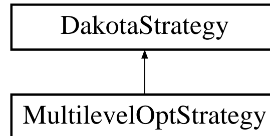
The documentation for this class was generated from the following files:

- MergedVariables.H
- MergedVariables.C

6.64 MultilevelOptStrategy Class Reference

Strategy for hybrid optimization using multiple optimizers on multiple models of varying fidelity.

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.

- const DakotaVariables & strategy_variable_results () const

  return the final solution from selectedIterators (variables).

- const DakotaResponse & strategy_response_results () const

  return the final solution from selectedIterators (response).

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.

6.64.1 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.

6.64.2 Member Function Documentation

6.64.2.1 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.

6.64.2.2 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.

6.64.2.3 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.

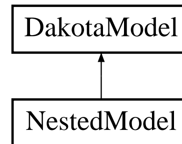
The documentation for this class was generated from the following files:

- MultilevelOptStrategy.H
- MultilevelOptStrategy.C

6.65 NestedModel Class Reference

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

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 DakotaResponseArray & derived_synchronize ()

    portion of synchronize() specific to NestedModel.

- const DakotaResponseList & 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.

- bool 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.

- DakotaResponseArray responseArray

  dummy response array for derived_synchronize() prior to derived_asynch_compute_response() support.

- DakotaResponseList 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.

6.65.1 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.

6.65.2 Member Function Documentation

6.65.2.1 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.

6.65.2.2 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.

6.65.2.3 const DakotaResponseArray & 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.

6.65.2.4 const DakotaResponseList & 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.

6.65.2.5 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.

6.65.2.6 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.

6.65.2.7 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.

6.65.3 Member Data Documentation

6.65.3.1 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.

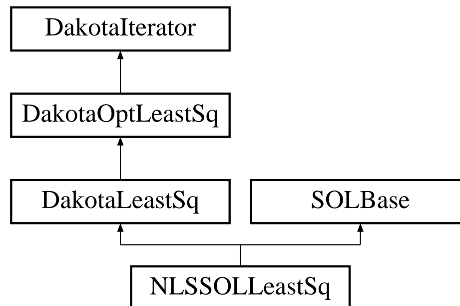
The documentation for this class was generated from the following files:

- NestedModel.H
- NestedModel.C

6.66 NLSSOLLeastSq Class Reference

Wrapper class for the NLSSOL nonlinear least squares library.

Inheritance diagram for NLSSOLLeastSq::



Public Methods

- NLSSOLLeastSq (DakotaModel &model)

  standard constructor.

- ~NLSSOLLeastSq ()

  destructor.

- void minimize_residuals ()

  Used within the least squares branch for minimizing the sum of squares residuals. Redefines the run_iterator virtual function for the least squares branch.

Static Private Methods

- void least_sq_eval (int &mode, int &m, int &n, int &nrowfj, Real ∗x, Real ∗f, Real ∗gradf, int &nstate)

  Evaluator for NLSSOL: computes the values and first derivatives of the least squares terms (passed by function pointer to NLSSOL).

6.66.1 Detailed Description

Wrapper class for the NLSSOL nonlinear least squares library.

The NLSSOLLeastSq class provides a wrapper for NLSSOL, a Fortran 77 sequential quadratic programming library from Stanford University marketed by Stanford Business Associates. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any 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 NLSSOLLeastSq's evaluator functions since there is no NLSSOL parameter equivalent, and `max_iterations`, `convergence_tolerance`, `output` verbosity, `verify_level`, `function_precision`, and `linesearch_tolerance` are mapped into NLSSOL's "Major Iteration Limit", "Optimality Tolerance", "Major Print Level" (`verbose`: Major Print Level = 20; `quiet`: Major Print Level = 10), "Verify Level", "Function Precision", and "Linesearch Tolerance" parameters, respectively, using NLSSOL's 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 NLSSOL's optional input parameters and the npoptn() subroutine.

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

- NLSSOLLeastSq.H
- NLSSOLLeastSq.C

6.67 NoDBBaseConstructor Struct Reference

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

Public Methods

- NoDBBaseConstructor (int=0)
  C++ structs can have constructors.

6.67.1 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.

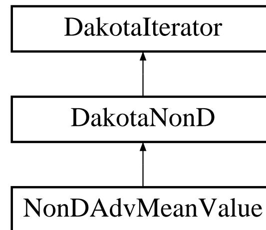
The documentation for this struct was generated from the following file:

- ProblemDescDB.H

6.68 NonDAdvMeanValue Class Reference

Class for the analytical reliability methods within DAKOTA/UQ.

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).

Private Methods

- void mean_value ()

  convenience function for encapsulating the simple Mean Value computation of approximate statistics and importance factors.

- void iterated_mean_value ()

  convenience function for encapsulating the iterated reliability methods (AMV, AMV+, FORM, SORM).

- 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.

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.

Private Attributes

- Epetra_SerialSymDenseMatrix petraCorrMatrix

  petra copy of uncertainCorrelations.

- 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.

- DakotaString reliabilityMethod

  reliability method identifier specified by user specifies amvFlag.

- DakotaRealMatrix impFactor

  importance factors predicted by MV.

- int numRelEqConstr

  number of equality constraints applied during the MPP search.

- size_t numLevels

  number of response/probaility levels to loop over.

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_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
  user specified targets for response levels.
- Epetra_SerialDenseVector petraProbLevels
  user specified targets for probability levels.
- Epetra_SerialDenseVector correctedRespLevel
  output response levels calculated.
- int respLevelCount
  counter for which response level is being analyzed.
- short 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.

6.68.1 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).

6.68.2 Member Function Documentation

6.68.2.1 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).

6.68.2.2 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).

6.68.2.3 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

6.68.2.4 void NonDAdvMeanValue::transXToU (const Epetra_SerialDenseVector & *random_vars*, Epetra_SerialDenseVector & *uncorr_normal_vars*) [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.

6.68.2.5 void NonDAdvMeanValue::transXToZ (const Epetra_SerialDenseVector & *random_vars*, Epetra_SerialDenseVector & *correlated_normal_vars*) [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.

6.68.2.6 void NonDAdvMeanValue::transUToZ (const Epetra_SerialDenseVector & *uncorr_normal_vars*, Epetra_SerialDenseVector & *correlated_normal_vars*) [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).

6.68.2.7 void NonDAdvMeanValue::transZToU (Epetra_SerialDenseVector & *correlated_normal_vars*, Epetra_SerialDenseVector & *uncorr_normal_vars*) [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).

6.68.2.8 void NonDAdvMeanValue::jacXToZ (const Epetra_SerialDenseVector & *random_vars*, const Epetra_SerialDenseVector & *correlated_normal_vars*, Epetra_SerialDenseMatrix & *jacobianXZ*) [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.

6.68.2.9 void NonDAdvMeanValue::jacZToX (const Epetra_SerialDenseVector & *correlated_normal_vars*, const Epetra_SerialDenseVector & *random_vars*, Epetra_SerialDenseMatrix & *jacobianZX*) [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.

6.68.2.10 void NonDAdvMeanValue::jacXToU (const Epetra_SerialDenseVector & *random_vars*, const Epetra_SerialDenseVector & *uncorr_normal_vars*, Epetra_SerialDenseMatrix & *jacobianXU*) [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.

6.68.2.11 void NonDAdvMeanValue::jacUToX (const Epetra_SerialDenseVector & *uncorr_normal_vars*, const Epetra_SerialDenseVector & *random_vars*, Epetra_SerialDenseMatrix & *jacobianUX*) [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.

6.68.2.12 void NonDAdvMeanValue::transNataf (Epetra_SerialSymDenseMatrix & *mod_corr_matrix*) [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.

6.68.3 Member Data Documentation

6.68.3.1 Epetra_SerialDenseVector NonDAdvMeanValue::correctedRespLevel [static, private]

output response levels calculated.

identical to petraRespLevels for AMV+/FORM, but will differ for AMV

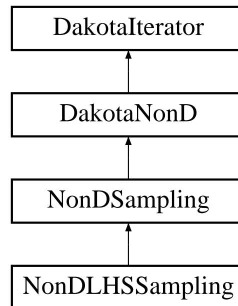
The documentation for this class was generated from the following files:

- NonDAdvMeanValue.H
- NonDAdvMeanValue.C

6.69 NonDLHSSampling Class Reference

Performs LHS and Monte Carlo sampling for uncertainty quantification.

Inheritance diagram for NonDLHSSampling::



Public Methods

- NonDLHSSampling (DakotaModel &model)

  constructor.

- NonDLHSSampling (DakotaModel &model, int samples, int seed, int num_vars, const DakotaRealVector &lower_bnds, const DakotaRealVector &upper_bnds)
- ∼NonDLHSSampling ()

  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.

Private Attributes

- bool allVarsFlag

  flags DACE mode using all variables.

6.69.1 Detailed Description

Performs LHS and Monte Carlo sampling for uncertainty quantification.

The Latin Hypercube Sampling (LHS) package from Sandia Albuquerque's Risk and Reliability organization provides comprehensive capabilities for Monte Carlo and Latin Hypercube sampling within a broad

array of user-specified probabilistic parameter distributions. It enforces user-specified rank correlations through use of a mixing routine. The NonDLHSSampling class provides a C++ wrapper for the LHS library and is used for performing forward propagations of parameter uncertainties into response statistics.

6.69.2 Constructor & Destructor Documentation

6.69.2.1 NonDLHSSampling::NonDLHSSampling (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.

6.69.2.2 NonDLHSSampling::NonDLHSSampling (DakotaModel & *model*, int *samples*, int *seed*, int *num_vars*, const DakotaRealVector & *lower_bnds*, const DakotaRealVector & *upper_bnds*)

This alternate constructor is used by ConcurrentStrategy for generation of uniform, uncorrelated sample sets. It is _not_ a letter-envelope instantiation and a set_db_list_nodes has not been performed. It is called with all needed data passed through the constructor and is designed to allow more flexibility in variables set definition (i.e., relax connection to a variables specification and allow sampling over parameter sets such as multiobjective weights). Data attributes taken from the model in the NoDBBaseConstructor constructors for DakotaNonD and DakotaIterator are not used, and other data attributes are not initialized and should not be avoided.

6.69.3 Member Function Documentation

6.69.3.1 void NonDLHSSampling::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 the set of samples and compute responses. Compute statistics on the set of responses if statsFlag is set.

Implements DakotaNonD.

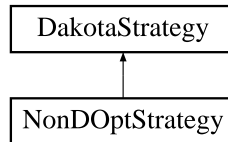
The documentation for this class was generated from the following files:

- NonDLHSSampling.H
- NonDLHSSampling.C

6.70 NonDOptStrategy Class Reference

Strategy for optimization under uncertainty (robust and reliability-based design).

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).

- const DakotaVariables & strategy_variable_results () const

  return the final solution from optIterator (variables).

- const DakotaResponse & strategy_response_results () const

  return the final solution from optIterator (response).

Private Attributes

- DakotaModel designModel

  the nested or layered model interfaced with optIterator.

- DakotaIterator optIterator

  the top level optimizer.

6.70.1 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().

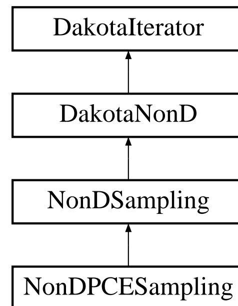
The documentation for this class was generated from the following files:

- NonDOptStrategy.H
- NonDOptStrategy.C

6.71 NonDPCESampling Class Reference

Stochastic finite element approach to uncertainty quantification using polynomial chaos expansions.

Inheritance diagram for NonDPCESampling::



Public Methods

- NonDPCESampling (DakotaModel &model)

  constructor.

- ∼NonDPCESampling ()

  destructor.

- void quantify_uncertainty ()

  perform a forward uncertainty propagation using SFEM/PCE methods.

- void print_iterator_results (ostream &s) const

  print the final statistics and PCE coefficient array.

Private Attributes

- DakotaRealVectorArray coeffArray

  Array containing Polynomial Chaos coefficients, one real vector per response function.

- int highestOrder

  Highest order of Hermite Polynomials in Expansion.

- int numChaos

  Number of terms in Polynomial Chaos Expansion.

6.71.1 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.

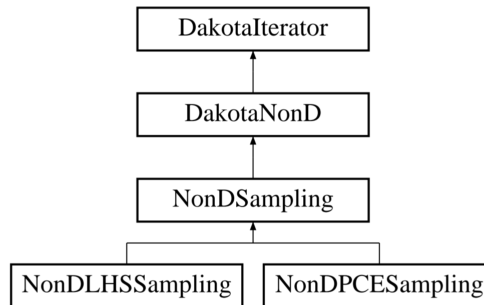
The documentation for this class was generated from the following files:

- NonDPCESampling.H
- NonDPCESampling.C

6.72 NonDSampling Class Reference

Base class for common code between NonDLHSSampling and NonDPCESampling.

Inheritance diagram for NonDSampling::



Public Methods

- NonDSampling (DakotaModel &model)

  constructor.

- NonDSampling (NoDBBaseConstructor, DakotaModel &model, int samples, int seed, int num_vars, const DakotaRealVector &lower_bnds, const DakotaRealVector &upper_bnds)
- ~NonDSampling ()

  destructor.

- void sampling_reset (int min_samples, bool all_data_flag, bool stats_flag)

  resets number of samples and sampling flags.

- const DakotaString & sampling_scheme () const

  return sampleType: "lhs" or "random".

Protected Methods

- void run_lhs ()

  generates the desired set of parameter samples from within user-specified probabilistic distributions. Supports both old and new LHS libraries. Used by NonDLHSSampling and NonDPCESampling.

- void compute_statistics (const DakotaRealVectorArray &samples)

  computes mean, standard deviation, and probability of failure for the samples input.

- void print_statistics (ostream &s) const

  prints the mean, standard deviation, and probability of failure statistics computed in compute_statistics().

Protected Attributes

- int numObservations

  the number of samples to evaluate.

- DakotaString sampleType

  the sample type: "lhs" or "random".

- bool statsFlag

  flags computation/output of statistics.

- bool 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).

Private Methods

- 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

- const int originalSeed

  the user seed specification (default is 0).

- int randomSeed

  the current random number seed.

- size_t numLHSRuns

  counter for number of executions of run_lhs() for this object.

- bool varyPattern

  flag for generating a sequence of seed values within multiple run_lhs() calls so that the run_lhs() executions (e.g., for surrogate-based optimization) are repeatable but not correlated.

- bool strategyFlag

  flag indicating a strategy other than "single_method". Used to deactivate some output when multiple sample sets may be generated.

6.72.1 Detailed Description

Base class for common code between NonDLHSSampling and NonDPCESampling.

This base class provides common code for sampling methods which employ the Latin Hypercube Sampling (LHS) package from Sandia Albuquerque's Risk and Reliability organization. NonDSampling manages two LHS versions within a ifdef construct in run_lhs(): (1) the 1998 Fortran 90 LHS version as documented in SAND98-0210, which was converted to a UNIX link library in 2001, (2) the 1970's vintage LHS that had been f2c'd and converted to (incomplete) classes.

6.72.2 Constructor & Destructor Documentation

6.72.2.1 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.

6.72.2.2 NonDSampling::NonDSampling (NoDBBaseConstructor, DakotaModel & *model*, int *samples*, int *seed*, int *num_vars*, const DakotaRealVector & *lower_bnds*, const DakotaRealVector & *upper_bnds*)

This alternate constructor is used by ConcurrentStrategy for generation of uniform, uncorrelated sample sets.

6.72.3 Member Function Documentation

6.72.3.1 void NonDSampling::sampling_reset (int *min_samples*, bool *all_data_flag*, bool *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.

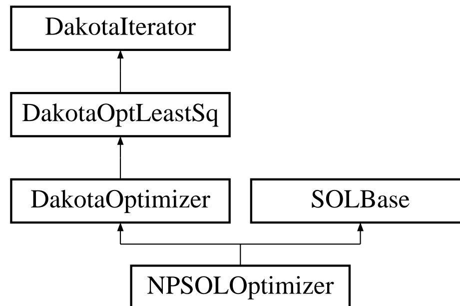
The documentation for this class was generated from the following files:

- NonDSampling.H
- NonDSampling.C

6.73 NPSOLOptimizer Class Reference

Wrapper class for the NPSOL optimization library.

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".

Static Private Methods

- void objective_eval (int &mode, int &n, Real *x, Real &f, Real *gradf, int &nstate)

  OBJFUN in NPSOL manual: computes the value and first derivatives of the objective function (passed by function pointer to NPSOL).

Private Attributes

- 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.

6.73.1 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

6.74 ParallelLibrary Class Reference

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

Public Methods

- ParallelLibrary (int &argc, char **&argv)

  constructor.

- ParallelLibrary ()

  default constructor.

- ParallelLibrary (int dummy)

  dummy constructor (used 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 manage_outputs_restart (CommandLineHandler &cmd_line_handler)

  manage output streams and restart file(s) using command line inputs (normal mode).

- void manage_outputs_restart (const char *clh_std_output_filename, const char *clh_std_error_filename, const char *clh_read_restart_filename, const char *clh_write_restart_filename, int restart_evals)

manage output streams and restart file(s) using external inputs (library mode).

- void close_streams ()

  close streams, files, and any other services.

- 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.
- bool mpirun_flag () const
  return mpirunFlag.
- Real parallel_time () const
  returns current MPI wall clock time.
- bool strategy_dedicated_master_flag () const
  return strategyDedicatedMasterFlag.
- bool strategy_iterator_split_flag () const
  return stratIteratorSplitFlag.
- bool iterator_master_flag () const
  return iteratorMasterFlag.
- bool strategy_iterator_message_pass () const
  return stratIteratorMessagePass.
- MPI_Comm iterator_intra_communicator () const
  return iteratorIntraComm.
- MPI_Comm strategy_iterator_intra_communicator () const
  return stratIteratorIntraComm.
- 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 strategy_iterator_communicator_rank () const
  return stratIteratorCommRank.
- int strategy_iterator_communicator_size () const
  return stratIteratorCommSize.
- int iterator_server_id () const
  return iteratorServerId.
- bool iterator_dedicated_master_flag () const
  return iteratorDedicatedMasterFlag.
- bool iterator_eval_split_flag () const
  return iteratorEvalSplitFlag.
- bool evaluation_master_flag () const
  return evalMasterFlag.
- bool iterator_eval_message_pass () const
  return iteratorEvalMessagePass.
- MPI_Comm evaluation_intra_communicator () const
  return evalIntraComm.
- MPI_Comm iterator_eval_intra_communicator () const
  return iteratorEvalIntraComm.
- 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 iterator_eval_communicator_rank () const
  return iteratorEvalCommRank.
- int iterator_eval_communicator_size () const
  return iteratorEvalCommSize.
- int evaluation_server_id () const

return evalServerId.

- bool evaluation_dedicated_master_flag () const

  return evalDedicatedMasterFlag.

- bool eval_analysis_split_flag () const

  return evalAnalysisSplitFlag.

- bool analysis_master_flag () const

  return analysisMasterFlag.

- bool eval_analysis_message_pass () const

  return evalAnalysisMessagePass.

- MPI_Comm analysis_intra_communicator () const

  return analysisIntraComm.

- MPI_Comm eval_analysis_intra_communicator () const

  return evalAnalysisIntraComm.

- 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 eval_analysis_communicator_rank () const

  return evalAnalysisCommRank.

- int eval_analysis_communicator_size () const

  return evalAnalysisCommSize.

- int analysis_server_id () const

  return analysisServerId.

Private Methods

- bool 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 &parent_child_intra_comm, int &parent_child_comm_rank, int &parent_child_comm_size, MPI_Comm &parent_child_inter_comm, MPI_Comm ∗&parent_child_inter_comms, int &server_id, bool &child_master_flag)

  split a parent communicator into a dedicated master processor and num_servers child communicators.

- bool 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 &parent_child_intra_comm, int &parent_child_comm_rank, int &parent_child_comm_size, MPI_Comm &parent_child_inter_comm, MPI_Comm ∗&parent_child_inter_comms, int &peer_id, bool &child_master_flag)

  split a parent communicator into num_servers child communicators (no dedicated master processor).

- bool 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

- ofstream output_ofstream

  tagged file redirection of stdout.

- ofstream error_ofstream

  tagged file redirection of stderr.

- int worldRank

  rank in MPI_COMM_WORLD.

- int worldSize

  size of MPI_COMM_WORLD.

- short parallelismLevels

  number of parallelism levels.

- bool mpirunFlag

  flag for a parallel mpirun/yod launch.

- bool ownMPIFlag

  flag for ownership of MPI_Init/MPI_Finalize.

- bool dummyFlag

  prevents multiple MPI_Finalize calls due to dummy_lib.

- bool stdOutputFlag

flags redirection of DAKOTA std output to a file.

- bool stdErrorFlag

  flags redirection of DAKOTA std error to a file.

- 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.

- bool strategyDedicatedMasterFlag

  signals ded. master partitioning.

- bool stratIteratorSplitFlag

  signals a communicator split was used.

- bool iteratorMasterFlag

  identifies master iterator processors.

- bool stratIteratorMessagePass

  flag for message passing at si level.

- MPI_Comm iteratorIntraComm

  intracomm for each iterator partition.

- MPI_Comm stratIteratorIntraComm

  intracomm for all iteratorCommRank==0 w/i MPI_COMM_WORLD.

- 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 stratIteratorCommRank
  rank in stratIteratorIntraComm.
- int stratIteratorCommSize
  size of stratIteratorIntraComm.
- int iteratorServerId
  identifier for an iterator server.
- bool iteratorDedicatedMasterFlag
  signals ded. master partitioning.
- bool iteratorEvalSplitFlag
  signals a communicator split was used.
- bool evalMasterFlag
  identifies master evaluation processors.
- bool iteratorEvalMessagePass
  flag for message passing at ie level.
- MPI_Comm evalIntraComm
  intracomm for each fn. eval. partition.
- MPI_Comm iteratorEvalIntraComm
  intracomm for all evalCommRank==0 w/i iteratorIntraComm.
- 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 iteratorEvalCommRank
  rank in iteratorEvalIntraComm.

- int iteratorEvalCommSize
  size of iteratorEvalIntraComm.
- int evalServerId
  identifier for an evaluation server.
- bool evalDedicatedMasterFlag
  signals dedicated master partitioning.
- bool evalAnalysisSplitFlag
  signals a communicator split was used.
- bool analysisMasterFlag
  identifies master analysis processors.
- bool evalAnalysisMessagePass
  flag for message passing at ea level.
- MPI_Comm analysisIntraComm
  intracomm for each analysis partition.
- MPI_Comm evalAnalysisIntraComm
  intracomm for all analysisCommRank==0 w/i evalIntraComm.
- 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 evalAnalysisCommRank
  rank in evalAnalysisIntraComm.
- int evalAnalysisCommSize
  size of evalAnalysisIntraComm.
- int analysisServerId
  identifier for an analysis server.

6.74.1 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.

6.74.2 Constructor & Destructor Documentation

6.74.2.1 ParallelLibrary::ParallelLibrary (int & *argc*, char **& *argv*)

constructor.

This constructor is the one used by main.C. It calls MPI_Init conditionally based on whether a parallel launch is detected.

6.74.2.2 ParallelLibrary::ParallelLibrary ()

default constructor.

This constructor provides a library mode and is used by the SIERRA Adak application. It does not call MPI_Init, but rather gathers data from MPI_COMM_WORLD if MPI_Init has been called elsewhere.

6.74.2.3 ParallelLibrary::ParallelLibrary (int *dummy*)

dummy constructor (used for dummy_lib).

This constructor is used for creation of the global dummy_lib object, which is used to satisfy initialization requirements when the real ParallelLibrary object is not available.

6.74.3 Member Function Documentation

6.74.3.1 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.

6.74.3.2 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().

6.74.3.3 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.

6.74.3.4 void ParallelLibrary::manage_outputs_restart (CommandLineHandler & *cmd_line_handler*)

manage output streams and restart file(s) using command line inputs (normal mode).

Get the -output, -error, -read_restart, and -write_restart filenames and the -stop_restart limit from the command line. Defaults for the filenames from the command line handler are NULL for the filenames and 0 for restart_evals if no user specification. Only worldRank==0 has access to command line arguments and must Bcast this data to all iterator masters.

6.74.3.5 void ParallelLibrary::manage_outputs_restart (const char * *clh_std_output_filename*, const char * *clh_std_error_filename*, const char * *clh_read_restart_filename*, const char * *clh_write_restart_filename*, int *restart_evals*)

manage output streams and restart file(s) using external inputs (library mode).

If the user has specified the use of files for DAKOTA standard output and/or standard error, then bind these filenames to the Cout/Cerr macros. In addition, if concurrent iterators are to be used, create and tag multiple output streams in order to prevent jumbled output. Manage restart file(s) by processing any incoming evaluations from an old restart file and by setting up the binary output stream for new evaluations.

Only master iterator processor(s) read & write restart information. This function must follow init_iterator_-communicators so that restart can be managed properly for concurrent iterator strategies. In the case of concurrent iterators, each iterator has its own restart file tagged with iterator number.

6.74.3.6 void ParallelLibrary::close_streams ()

close streams, files, and any other services.

Close streams associated with manage_outputs and manage_restart and terminate any additional services that may be active.

6.74.3.7 bool 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

6.75 ParamResponsePair Class Reference

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

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

- bool operator== (const ParamResponsePair &pair1, const ParamResponsePair &pair2)

  equality operator.

- bool operator!= (const ParamResponsePair &pair1, const ParamResponsePair &pair2)

  inequality operator.

6.75.1 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.

6.75.2 Constructor & Destructor Documentation

6.75.2.1 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).

6.75.2.2 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.

6.75.3 Member Data Documentation

6.75.3.1 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.

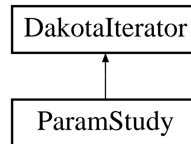
The documentation for this class was generated from the following files:

- ParamResponsePair.H
- ParamResponsePair.C

6.76 ParamStudy Class Reference

Class for vector, list, centered, and multidimensional parameter studies.

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 ¤t_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.

- bool nestedFlag

  flag set by parameter studies which call other parameter studies in loops.

- 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.

- int psCounter

  class-scope counter (needed for asynchronous multidim_loop).

6.76.1 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.

6.76.2 Member Function Documentation

6.76.2.1 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

6.77 ProblemDescDB Class Reference

The database containing information parsed from the DAKOTA input file.

Public Methods

- ProblemDescDB (ParallelLibrary ¶llel_lib)

  constructor.

- ∼ProblemDescDB ()

  destructor.

- void manage_inputs (int argc, char **argv, CommandLineHandler &cmd_line_handler)

  parses the input file and populates the problem description database. This version reads from the dakota input filename passed with the "-input" option on the DAKOTA command line.

- void manage_inputs (const char *dakota_input_file)

  parses the input file and populates the problem description database. This version reads from the dakota input filename passed in.

- void check_input ()

  verifies that there was at least one of each of the required keywords in the dakota input file. Used by manage_inputs().

- void set_db_list_nodes (const DakotaString &method_tag)

  set methodIter 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 iterators.

- void set_db_list_nodes (const size_t &method_index)

  set methodIter based on the active index to activate a particular method specification in methodList and use pointers from this method specification to set the other list iterators.

- size_t get_db_list_nodes () const

  return the index of the active node in methodList.

- void set_db_interface_node (const DakotaString &interface_tag)

  set interfaceIter based on the interface identifier string.

- void set_db_responses_node (const DakotaString &responses_tag)

  set responsesIter based on the responses identifier string.

- void set_db_model_type (const DakotaString &model_type)

  set the model type.

- 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 DakotaRealVectorArray & get_drva (const DakotaString &entry_name) const
  get a DakotaRealVectorArray 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 bool & get_bool (const DakotaString &entry_name) const
  get a bool out of the database based on an identifier string.
- void insert_node (const DataStrategy &data_strategy)
  set the DataStrategy object.
- void insert_node (const DataMethod &data_method)
  add a DataMethod object to the methodList.
- void insert_node (const DataVariables &data_variables)
  add a DataVariables object to the variablesList.

- void insert_node (const DataInterface &data_interface)

  add a DataInterface object to the interfaceList.

- void insert_node (const DataResponses &data_responses)

  add a DataResponses object to the responsesList.

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 send_db_buffer ()

  MPI send of a large buffer containing strategy specification attributes and all the objects in interfaceList, variablesList, methodList, and responsesList. Used by manage_inputs().

- void receive_db_buffer ()

  MPI receive of a large buffer containing strategy specification attributes and all the objects in interfaceList, variablesList, methodList, and responsesList. Used by manage_inputs().

- void set_other_list_nodes ()

  convenience function used by set_db_list_nodes(method_tag) and set_db_list_nodes(method_index) to set the other list iterators once methodIter 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 for each entry in label_array. Uses build_label().

- void build_labels_partial (DakotaStringArray &label_array, const DakotaString &root_label, size_t start_index, size_t num_items)

  create a partial array of labels by tagging root_label for a subset of entries in label_array. Uses build_label().

Private Attributes

- DakotaList< DataMethod >::iterator methodIter

  iterator identifying the active list node in methodList.

- DakotaList< DataVariables >::iterator variablesIter

  iterator identifying the active list node in variablesList.

- DakotaList< DataInterface >::iterator interfaceIter

  iterator identifying the active list node in interfaceList.

- DakotaList< DataResponses >::iterator responsesIter

  iterator identifying the active list node in responsesList.

- bool dbLocked

  prevents use of get_<type> data retrieval functions prior to a set_db_list_nodes invocation.

- ParallelLibrary & parallelLib

  reference to the parallel_lib object passed from main.

Static Private Attributes

- DataStrategy strategySpec

  the strategy specification (only one allowed) resulting from a call to strategy_kwhandler() or insert_node().

- DakotaList< DataMethod > methodList

  list of method specifications, one for each call to method_kwhandler() or insert_node().

- DakotaList< DataVariables > variablesList

  list of variables specifications, one for each call to variables_kwhandler() or insert_node().

- DakotaList< DataInterface > interfaceList

  list of interface specifications, one for each call to interface_kwhandler() or insert_node().

- DakotaList< DataResponses > responsesList

  list of responses specifications, one for each call to responses_kwhandler() or insert_node().

- size_t strategyCntr

  counter for strategy specifications used in check_input.

6.77.1 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

6.77.2 Member Function Documentation

6.77.2.1 void ProblemDescDB::manage_inputs (int *argc*, char ** *argv*, CommandLineHandler & *cmd_line_handler*)

parses the input file and populates the problem description database. This version reads from the dakota input filename passed with the "-input" option on the DAKOTA command line.

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.

6.77.2.2 void ProblemDescDB::manage_inputs (const char * *dakota_input_file*)

parses the input file and populates the problem description database. This version reads from the dakota input filename passed in.

Parse the input file using the Input Deck Reader (IDR) parsing system. IDR populates the ProblemDescDB object with the input file data.

6.77.2.3 void ProblemDescDB::set_db_model_type (const DakotaString & *model_type*) `[inline]`

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.

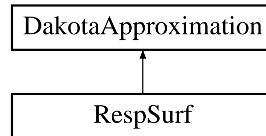
The documentation for this class was generated from the following files:

- ProblemDescDB.H
- ProblemDescDB.C

6.78 RespSurf Class Reference

Derived approximation class for polynomial regression.

Inheritance diagram for RespSurf::



Public Methods

- RespSurf (const ProblemDescDB &problem_db, const size_t &num_acv)

  constructor.

- ∼RespSurf ()

  destructor.

Protected Methods

- void find_coefficients ()

  Least squares fit to data using a singular value decomposition.

- int required_samples ()

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

- const DakotaRealVector & approximation_coefficients ()

  return the coefficient array computed by find_coefficients().

- 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 numCoeffs

  number of coefficients used by the polynomial model.

- DakotaRealVector polyCoeffs

vector of polynomial coefficients.

- int polyOrder

  flag to indicate a linear (value=1), quadratic (value = 2), or cubic (value = 3) polynomial model.

6.78.1 Detailed Description

Derived approximation class for polynomial regression.

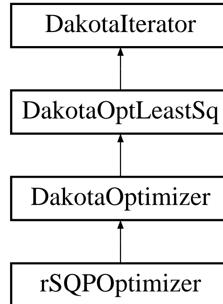
The RespSurf class computes a linear, quadratic, or cubic polynomial fit to data. The polynomial has either n+1 (linear case), (n+1)*(n+2)/2 (quadratic case), or (n^3+6n^2+11n+6)/6 (cubic case) coefficients for n variables. A least squares estimation of the polynomial coefficients is performed using 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

6.79 rSQPOptimizer Class Reference

Inheritance diagram for rSQPOptimizer::



Public Methods

- **rSQPOptimizer** (DakotaModel &model)
- ~**rSQPOptimizer** ()
- int **num_objectives** () const
- const DakotaRealVector & **lin_ineq_lb** () const
- const DakotaRealVector & **lin_ineq_ub** () const
- const DakotaRealVector & **nonlin_ineq_lb** () const
- const DakotaRealVector & **nonlin_ineq_ub** () const
- const DakotaRealVector & **lin_eq_targ** () const
- const DakotaRealVector & **nonlin_eq_targ** () const
- const DakotaRealMatrix & **lin_eq_jac** () const
- const DakotaRealMatrix & **lin_ineq_jac** () const

Overridden from DakotaOptimizer

- void find_optimum ()
  Used within the optimizer branch for computing the optimal solution. Redefines the run_iterator virtual function for the optimizer branch.

Private Attributes

- DakotaModel ∗ **model_**
- NLPInterfacePack::NLPDakota **nlp_**

6.79.1 Detailed Description

Wrapper class for the rSQP++ optimization library.

The rSQPOptimizer class provides a wrapper for rSQP++, a C++ sequential quadratic programming library written by Roscoe Bartlett. rSQP++ can currently be used in NAND mode, although use of its SAND

mode for reduced-space SQP is planned. rSQPOptimizer uses a NLPDakota object to perform the function evaluations.

The user input mappings will ultimately include: `max_iterations`, `convergence_tolerance`, `output_verbosity`.

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

- rSQPOptimizer.H
- rSQPOptimizer.C

6.80 SGOPTApplication Class Reference

Maps the evaluation functions used by SGOPT algorithms to the DAKOTA evaluation functions.

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 bool &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.

- bool dakotaModelAsynchFlag

  a flag for asynchronous DAKOTA evaluations.

- DakotaResponseList 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.

6.80.1 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.

6.80.2 Member Function Documentation

6.80.2.1 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).

6.80.2.2 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.

6.80.2.3 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.

6.80.2.4 void SGOPTApplication::dakota_asynch_flag (const bool & *asynch_flag*) [inline]

set dakotaModelAsynchFlag.

This function is needed to publish the iterator's asynchFlag at run time (asynchFlag not available at construction).

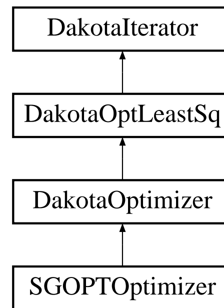
The documentation for this class was generated from the following files:

- SGOPTApplication.H
- SGOPTApplication.C

6.81 SGOPTOptimizer Class Reference

Wrapper class for the SGOPT optimization library.

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.

- bool 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.

6.81.1 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.

6.81.2 Constructor & Destructor Documentation

6.81.2.1 SGOPTOptimizer::SGOPTOptimizer (DakotaModel & *model*)

constructor.

The constructor allocates the objects and populates the class member pointer attributes.

6.81.2.2 SGOPTOptimizer::∼SGOPTOptimizer ()

destructor.

The destructor deallocates the class member pointer attributes.

6.81.3 Member Function Documentation

6.81.3.1 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.

Implements DakotaOptimizer.

6.81.3.2 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.

6.81.4 Member Data Documentation

6.81.4.1 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.

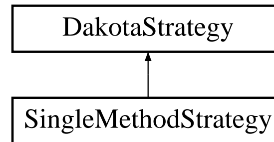
The documentation for this class was generated from the following files:

- SGOPTOptimizer.H
- SGOPTOptimizer.C

6.82 SingleMethodStrategy Class Reference

Simple fall-through strategy for running a single iterator on a single model.

Inheritance diagram for SingleMethodStrategy::



Public Methods

- SingleMethodStrategy (ProblemDescDB &problem_db)
  constructor.
- ~SingleMethodStrategy ()
  destructor.
- void run_strategy ()
  Perform the strategy by executing selectedIterator on userDefinedModel.
- const DakotaVariables & strategy_variable_results () const
  return the final solution from selectedIterator (variables).
- const DakotaResponse & strategy_response_results () const
  return the final solution from selectedIterator (response).

Private Attributes

- DakotaModel userDefinedModel
  the model to be iterated.
- DakotaIterator selectedIterator
  the iterator.

6.82.1 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.

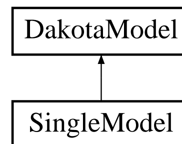
The documentation for this class was generated from the following files:

- SingleMethodStrategy.H
- SingleMethodStrategy.C

6.83 SingleModel Class Reference

Derived model class which utilizes a single interface to map variables into responses.

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 userDefined-Interface).

- void derived_asynch_compute_response (const DakotaIntArray &asv)

  portion of asynch_compute_response() specific to SingleModel (invokes an asynchronous map() on user-DefinedInterface).

- const DakotaResponseArray & derived_synchronize ()

  portion of synchronize() specific to SingleModel (invokes synch() on userDefinedInterface).

- const DakotaResponseList & 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 userDefined-Interface).

- bool derived_master_overload () const

  flag which prevents overloading the master with a multiprocessor evaluation (request forwarded to user-DefinedInterface).

- 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.

6.83.1 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.

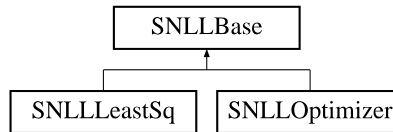
The documentation for this class was generated from the following files:

- SingleModel.H
- SingleModel.C

6.84 SNLLBase Class Reference

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

Inheritance diagram for SNLLBase::



Public Methods

- SNLLBase ()

  default constructor.

- SNLLBase (DakotaModel &model)

  standard constructor.

- ~SNLLBase ()

  destructor.

Protected Methods

- void pre_instantiate (const DakotaString &merit_fn, bool bound_constr_flag, const int &num_constr)

  convenience function for setting OPT++ options prior to the method instantiation.

- void post_instantiate (const int &num_cv, bool vendor_num_grad_flag, const DakotaString &finite_-diff_type, const Real &fdss, const int &max_iter, const int &max_fn_evals, const Real &conv_tol, const Real &grad_tol, const Real &max_step, bool bound_constr_flag, const int &num_constr, bool debug_output, OptimizeClass ∗the_optimizer, NLP0 ∗nlf_objective, FDNLF1 ∗fd_nlf1, FDNLF1 ∗fd_nlf1_con)

  convenience function for setting OPT++ options after the method instantiation.

- void pre_run (NLP0 ∗nlf_objective, NLP ∗nlp_constraint, const DakotaModel &model, bool bound_constr_flag, const DakotaRealVector &nln_ineq_l_bnds, const DakotaRealVector &nln_ineq_-u_bnds, const DakotaRealVector &nln_eq_targets)

  convenience function for OPT++ configuration prior to the method invocation.

- void post_run (NLP0 ∗nlf_objective, DakotaVariables &best_vars)

  convenience function for setting OPT++ options after the method instantiations.

Static Protected Methods

- void init_fn (int n, ColumnVector &x)

  An initialization mechanism provided by OPT++ (not currently used).

- void copy_con_vals (const DakotaRealVector &local_fn_vals, ColumnVector &g, const size_t &offset)

  convenience function for copying local_fn_vals to g; used by constraint evaluator functions.

- void copy_con_vals (const ColumnVector &g, DakotaRealVector &local_fn_vals, const size_t &offset)

  convenience function for copying g to local_fn_vals; used in final solution logging.

- void copy_con_grad (const DakotaRealMatrix &local_fn_grads, Matrix &grad_g, const size_t &offset)

  convenience function for copying local_fn_grads to grad_g; used by constraint evaluator functions.

- void copy_con_hess (const DakotaRealMatrixArray &local_fn_hessians, OptppArray< SymmetricMatrix > &hess_g, const size_t &offset)

  convenience function for copying local_fn_hessians to hess_g; used by constraint evaluator functions.

Protected 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.

- bool constantASVFlag

  flags a user selection of active_set_vector == constant. By mapping this into mode override, reliance on duplicate detection can be avoided.

Static Protected Attributes

- EvalType staticLastFnEvalLocn

  an enum used to track whether an nlf evaluator or a constraint evaluator was the last location of a function evaluation.

- bool staticDebugOutput

  static copy of debugOutput.

- bool staticModeOverrideFlag

  flags OPT++ mode override (for combining value, gradient, and Hessian requests).

- int staticConEvalMode

  static copy of mode from constraint evaluators.

- DakotaRealVector staticConEvalVars

  static copy of variables from constraint evaluators.

- int staticNumNonlinearEqConstraints

  number of nonlinear equality constraints.

- int staticNumNonlinearIneqConstraints

  number of nonlinear inequality constraints.

6.84.1 Detailed Description

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

The SNLLBase class provides a common base class for SNLLOptimizer and SNLLLeastSq, both of which are wrappers for OPT++, a C++ optimization library from the Computational Sciences and Mathematics Research (CSMR) department at Sandia's Livermore CA site.

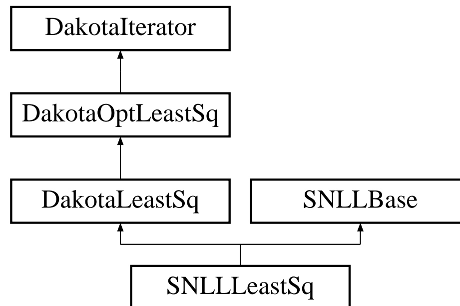
The documentation for this class was generated from the following files:

- SNLLBase.H
- SNLLBase.C

6.85 SNLLLeastSq Class Reference

Wrapper class for the OPT++ optimization library.

Inheritance diagram for SNLLLeastSq::



Public Methods

- SNLLLeastSq (DakotaModel &model)

  constructor.

- ~SNLLLeastSq ()

  destructor.

- void minimize_residuals ()

  Performs the iterations to determine the least squares solution.

Static Private Methods

- void nlf2_evaluator_gn (int mode, int n, const ColumnVector &x, Real &f, ColumnVector &grad_f, SymmetricMatrix &hess_f, int &result_mode)

  objective function evaluator function which obtains values and gradients for least square terms and computes objective function value, gradient, and Hessian using the Gauss-Newton approximation.

- void constraint2_evaluator_gn (int mode, int n, const ColumnVector &x, ColumnVector &g, Matrix &grad_g, OptppArray< SymmetricMatrix > &hess_g, int &result_mode)

  constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ Gauss-Newton methods. While it does not employ the Gauss-Newton approximation, it is distinct from constraint2_evaluator() due to its need to anticipate the required modes for the least squares terms.

Private Attributes

- NLP0 ∗ nlfObjective

  objective NLF base class pointer.

- NLP0 * nlfConstraint

  constraint NLF base class pointer.

- NLP * nlpConstraint

  constraint NLP pointer.

- NLF2 * nlf2

  pointer to objective NLF for full Newton optimizers.

- NLF2 * nlf2Con

  pointer to constraint NLF for full Newton optimizers.

- OptimizeClass * theOptimizer

  optimizer base class pointer.

- OptNewton * optnewton

  Newton optimizer pointer.

- OptBCNewton * optbcnewton

  Bound constrained Newton optimizer pointer.

- OptNIPS * optnips

  NIPS optimizer pointer.

6.85.1 Detailed Description

Wrapper class for the OPT++ optimization library.

The SNLLLeastSq class provides a wrapper for OPT++, a C++ optimization library of nonlinear programming and pattern search techniques from the Computational Sciences and Mathematics Research (CSMR) department at Sandia's Livermore CA site. It uses a function pointer approach for which passed functions must be either global functions or static member functions. Any attribute used within static member functions must be either local to that function 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`, and `search_scheme_size` are set using OPT++'s setMaxIter(), setMaxFeval(), setFcnTol(), setMaxStep(), setGradTol(), setSearchStrategy(), and setSSS() member functions, respectively; `output` verbosity is used to toggle OPT++'s debug mode using the setDebug() member function. Internal to OPT++, there are 3 search strategies, while the DAKOTA `search_method` specification supports 4 (`value_based_line_search`, `gradient_based_line_search`, `trust_region`, or `tr_pds`). The difference stems from the "is_expensive" flag in OPT++. If the search strategy is LineSearch and "is_expensive" is turned on, then the `value_based_line_search` is used. Otherwise (the "is_expensive" default is off), the algorithm will use the `gradient_based_line_search`. Refer to [Meza, J.C., 1994] and to the OPT++ source in the Dakota/VendorOptimizers/opt++ directory for information on OPT++ class member functions.

6.85.2 Member Function Documentation

6.85.2.1 void SNLLLeastSq::nlf2_evaluator_gn (int *mode*, int *n*, const ColumnVector & *x*, Real & *f*, ColumnVector & *grad_f*, SymmetricMatrix & *hess_f*, int & *result_mode*) `[static, private]`

objective function evaluator function which obtains values and gradients for least square terms and computes objective function value, gradient, and Hessian using the Gauss-Newton approximation.

This nlf2 evaluator function is used for the Gauss-Newton method in order to exploit the special structure of the nonlinear least squares problem. Here, fx = sum (T_i - Tbar_i)^2 and DakotaResponse is made up of residual functions and their gradients along with any nonlinear constraints. The objective function and its gradient vector and Hessian matrix are computed directly from the residual functions and their derivatives (which are returned from the DakotaResponse object).

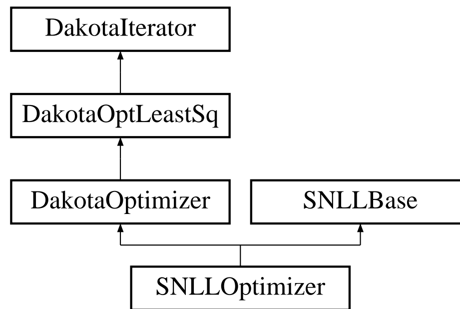
The documentation for this class was generated from the following files:

- SNLLLeastSq.H
- SNLLLeastSq.C

6.86 SNLLOptimizer Class Reference

Wrapper class for the OPT++ optimization library.

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 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 nlf1_evaluator (int mode, int n, const ColumnVector &x, Real &f, ColumnVector &grad_f, 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 &grad_f, SymmetricMatrix &hess_f, int &result_mode)

  objective function evaluator function which provides function values, gradients, and Hessians to OPT++ methods.

- void constraint0_evaluator (int n, const ColumnVector &x, ColumnVector &g, 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 &g, Matrix &grad_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 &g, Matrix &grad_g, OptppArray< SymmetricMatrix > &hess_g, int &result_mode)

  constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ methods.

Private Attributes

- 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-based optimizers.

- NLF1 * nlf1Con

  pointer to constraint NLF for (analytic) gradient-based optimizers.

- FDNLF1 * fdnlf1

  pointer to objective NLF for (finite diff) gradient-based optimizers.

- FDNLF1 * fdnlf1Con

  pointer to constraint NLF for (finite diff) gradient-based optimizers.

- NLF2 * nlf2

  pointer to objective NLF for full Newton optimizers.

- NLF2 * nlf2Con

  pointer to constraint NLF for 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

  Bnd constrained Quasi-Newton optimizer ptr.

- OptBCFDNewton * optbcfdnewton

  Bnd constrained FD-Newton optimizer ptr.

- OptNIPS * optnips

  NIPS optimizer pointer.

- OptQNIPS * optqnips

  Quasi-Newton NIPS optimizer pointer.

- OptFDNIPS * optfdnips

  Finite Difference NIPS optimizer pointer.

6.86.1 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`, and `search_scheme_size` are set using OPT++'s setMaxIter(), setMaxFeval(), setFcnTol(), setMaxStep(), setGradTol(), setSearchStrategy(), and setSSS() member functions, respectively; `output` verbosity is used to toggle OPT++'s debug mode using the setDebug() member function. Internal to OPT++, there are 3 search strategies, while the DAKOTA `search_method` specification supports 4 (`value_based_line_search`, `gradient_based_line_search`, `trust_region`, or `tr_pds`). The difference stems from the "is_expensive" flag in OPT++. If the search strategy is LineSearch and "is_expensive" is turned on, then the `value_based_line_search` is used. Otherwise (the "is_expensive" default is off), the algorithm will use the `gradient_based_line_search`. Refer to [Meza, J.C., 1994] and to the OPT++ source in the Dakota/VendorOptimizers/opt++ directory for information on OPT++ class member functions.

6.86.2 Member Function Documentation

6.86.2.1 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 gradients are not directly available. This is used by nongradient-based optimizers such as PDS and by gradient-based optimizers in vendor numerical gradient mode (opt++'s internal finite difference routine is used).

6.86.2.2 void SNLLOptimizer::nlf1_evaluator (int *mode*, int *n*, const ColumnVector & *x*, Real & *f*, ColumnVector & *grad_f*, int & *result_mode*) `[static, private]`

objective function evaluator function which provides function values and gradients to OPT++ methods.

For use when DAKOTA computes f and df/dX (regardless of gradientType). Vendor numerical gradient case is handled by nlf0_evaluator.

6.86.2.3 void SNLLOptimizer::nlf2_evaluator (int *mode*, int *n*, const ColumnVector & *x*, Real & *f*, ColumnVector & *grad_f*, SymmetricMatrix & *hess_f*, int & *result_mode*) `[static, private]`

objective function evaluator function which provides function values, gradients, and Hessians to OPT++ methods.

For use when DAKOTA receives f, df/dX, & d^2f/dx^2 from the ApplicationInterface (analytic only). Finite differencing does not make sense for a full Newton approach, since lack of analytic gradients & Hessian should dictate the use of quasi-newton or fd-newton. Thus, there is no fdnlf2_evaluator for use with full Newton approaches, since it is preferable to use quasi-newton or fd-newton with nlf1. Gauss-Newton does not fit this model; it uses nlf2_evaluator_gn instead of nlf2_evaluator.

6.86.2.4 void SNLLOptimizer::constraint0_evaluator (int *n*, const ColumnVector & *x*, ColumnVector & *g*, int & *result_mode*) `[static, private]`

constraint evaluator function for OPT++ methods which require only constraint values.

For use when DAKOTA computes g and gradients are not directly available. This is used by nongradient-based optimizers and by gradient-based optimizers in vendor numerical gradient mode (opt++'s internal finite difference routine is used).

6.86.2.5 void SNLLOptimizer::constraint1_evaluator (int *mode*, int *n*, const ColumnVector & *x*, ColumnVector & *g*, Matrix & *grad_g*, int & *result_mode*) `[static, private]`

constraint evaluator function which provides constraint values and gradients to OPT++ methods.

For use when DAKOTA computes g and dg/dX (regardless of gradientType). Vendor numerical gradient case is handled by constraint0_evaluator.

6.86.2.6 void SNLLOptimizer::constraint2_evaluator (int *mode*, int *n*, const ColumnVector & *x*, ColumnVector & *g*, Matrix & *grad_g*, OptppArray< SymmetricMatrix > & *hess_g*, int & *result_mode*) `[static, private]`

constraint evaluator function which provides constraint values, gradients, and Hessians to OPT++ methods.

For use when DAKOTA computes g, dg/dX, & d^2g/dx^2 (analytic only).

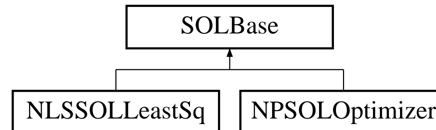
The documentation for this class was generated from the following files:

- SNLLOptimizer.H
- SNLLOptimizer.C

6.87 SOLBase Class Reference

Base class for Stanford SOL software.

Inheritance diagram for SOLBase::



Public Methods

- SOLBase ()

  default constructor.

- SOLBase (DakotaModel &model)

  standard constructor.

- ∼SOLBase ()

  destructor.

Protected Methods

- void allocate_arrays (const int &num_cv, const size_t &num_nln_ineq_con, const size_t &num_nln_eq_con, const size_t &num_lin_ineq_con, const size_t &num_lin_eq_con, const DakotaRealMatrix &lin_ineq_coeffs, const DakotaRealMatrix &lin_eq_coeffs)

  Allocates miscellaneous arrays for the SOL algorithms.

- void deallocate_arrays ()

  Deallocates memory previously allocated by allocate_arrays().

- void allocate_workspace (const int &num_cv, const int &num_nln_con, const int &num_lin_con, const int &num_lsq)

  Allocates real and integer workspaces for the SOL algorithms.

- void set_options (bool speculative_flag, bool vendor_num_grad_flag, bool verbose_output, const int &verify_lev, const Real &fn_prec, const Real &linesrch_tol, const int &max_iter, const Real &constr_tol, const Real &conv_tol, const DakotaString &grad_type, const Real &fdss)

  Sets SOL method options using calls to npoptn2.

- void augment_bounds (DakotaRealVector &augmented_l_bnds, DakotaRealVector &augmented_u_bnds, const DakotaRealVector &lin_ineq_l_bnds, const DakotaRealVector &lin_ineq_u_bnds, const DakotaRealVector &lin_eq_targets, const DakotaRealVector &nln_ineq_l_bnds, const DakotaRealVector &nln_ineq_u_bnds, const DakotaRealVector &nln_eq_targets)

augments variable bounds with linear and nonlinear constraint bounds.

Static Protected Methods

- void constraint_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.

Protected Attributes

- int realWorkSpaceSize

  size of realWorkSpace.

- int intWorkSpaceSize

  size of intWorkSpace.

- DakotaRealArray realWorkSpace

  real work space for NPSOL/NLSSOL.

- DakotaIntArray intWorkSpace

  int work space for NPSOL/NLSSOL.

- int nlnConstraintArraySize

  used for non-zero array sizing (nonlinear constraints).

- int linConstraintArraySize

  used for non-zero array sizing (linear constraints).

- 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.

Static Protected Attributes

- int fnEvalCntr

  counter for testing against staticMaxFnEvals.

- size_t staticConstrOffset

  used in constraint_eval() to bridge NLSSOLLeastSq::numLeastSqTerms and NPSOLOptimizer::numObjectiveFunctions.

- DakotaModel & staticSOLModel = dummy_model

  static reference to userDefinedModel used in constraint_eval().

- int staticMaxFnEvals

  static copy of DakotaIterator::maxFunctionEvals.

- int staticVendorNumericalGradFlag

  static copy of DakotaOptimizer::vendorNumericalGradFlag.

6.87.1 Detailed Description

Base class for Stanford SOL software.

The SOLBase class provides a common base class for NPSOLOptimizer and NLSSOLLeastSq, both of which are Fortran 77 sequential quadratic programming algorithms from Stanford University marketed by Stanford Business Associates.

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

- SOLBase.H
- SOLBase.C

6.88 SortCompare Class Template Reference

Public Methods

- SortCompare (bool(∗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

- bool(∗ sortFunction)(const T &, const T &)

  Pointer to test function.

6.88.1 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.

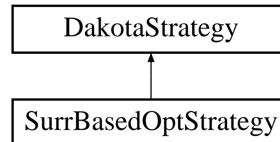
The documentation for this class was generated from the following file:

- DakotaList.H

6.89 SurrBasedOptStrategy Class Reference

Strategy for provably-convergent surrogate-based optimization.

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.

- const DakotaVariables & strategy_variable_results () const

  return the SBO final solution (variables).

- const DakotaResponse & strategy_response_results () const

  return the SBO final solution (response).

Private Methods

- Real compute_penalty_function (const DakotaRealVector &fn_vals)

  compute a penalty function from a set of function values.

- void hard_convergence_check (const DakotaResponse &response_center_truth)

  check for hard convergence (zero gradient of penalty function).

- void 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.

- DakotaRealVector trustRegionSize

  the size of the current trust region is computed my multiplying the trustRegionFactor value by the difference between the lower and upper bounds.

- Real trustRegionFactor

  the trust region factor is used to compute the size of the trust region – it is a percentage, e.g. for trustRegion-Factor = 0.1 the actual size of the trust region will be 10% of the global bounds (upper bound - lower bound for each design variable).

- Real minTrustRegionFactor

  a soft convergence control: stop SBO when the trust region factor is reduced below the value of minTrust-RegionFactor.

- 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 exponen-tially with iteration count.

- Real trRatioContractValue

  trust region ratio min value: contract tr if ratio below this value.

- Real trRatioExpandValue

  trust region ratio sufficient value: expand tr if ratio above this value.

- Real gammaContract

  trust region contraction factor.

- Real gammaExpand

  trust region expansion factor.

- Real gammaNoChange

  factor for maintaining the current trust region size (normally 1.0).

- int iterMax

  maximum number of SBO iterations.

- short convergenceFlag

code indicating satisfaction of hard or soft convergence conditions.

- int numFns

  number of response functions.

- int numVars

  number of active continuous variables.

- short softConvCount

  number of consecutive candidate point rejections. If the count reaches softConvLimit, stop SBO.

- short softConvLimit

  the limit on consecutive candidate point rejections. If exceeded by softConvCount, stop SBO.

- bool gradientFlag

  flags the use of gradients throughout the SBO process.

- bool correctionFlag

  flags the use of surrogate correction techniques at the center of each trust region.

- bool globalApproxFlag

  flags the use of a global data fit surrogate (rsm, ann, mars, kriging).

- bool localApproxFlag

  flags the use of a local data fit surrogate (Taylor series).

- bool hierarchApproxFlag

  flags the use of a hierarchical surrogate.

- bool newCenterFlag

  flags the acceptance of a candidate point and the existence of a new trust region center.

- bool 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.

- DakotaVariables bestVariables

  best variables found in SBO.

- DakotaResponse bestResponses

  best responses found in SBO.

6.89.1 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.

6.89.2 Member Function Documentation

6.89.2.1 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.

6.89.2.2 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.

6.89.2.3 void SurrBasedOptStrategy::hard_convergence_check (const DakotaResponse & *response_center_truth*) `[private]`

check for hard convergence (zero gradient of penalty function).

The hard convergence check computes the 2-norm of the gradient of the penalty function at the trust region center and signals convergence if the 2-norm is close to zero.

6.89.2.4 void 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 (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).

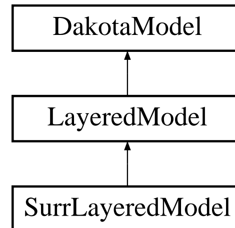
The documentation for this class was generated from the following files:

- SurrBasedOptStrategy.H
- SurrBasedOptStrategy.C

6.90 SurrLayeredModel Class Reference

Derived model class within the layered model branch for managing data fit surrogates (global and local).

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 DakotaResponseArray & derived_synchronize ()

  portion of synchronize() specific to SurrLayeredModel.

- const DakotaResponseList & derived_synchronize_nowait ()

  portion of synchronize_nowait() specific to SurrLayeredModel.

- bool 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).

- const DakotaRealVectorArray & approximation_coefficients ()

  return the approximation coefficients from each DakotaApproximation (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

  string identifier for the actual interface from the local approximation specification (required for local); used to build actualModel for local approximations.

- DakotaString daceMethodPointer

  string identifier for 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).

6.90.1 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.

6.90.2 Member Function Documentation

6.90.2.1 void SurrLayeredModel::derived_compute_response (const DakotaIntArray & *asv*) [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.

6.90.2.2 void SurrLayeredModel::derived_asynch_compute_response (const DakotaIntArray & *asv*) [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 bookkeeps the results for return in derived_synchronize() below).

Reimplemented from DakotaModel.

6.90.2.3 const DakotaResponseArray & SurrLayeredModel::derived_synchronize () [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.

6.90.2.4 const DakotaResponseList & SurrLayeredModel::derived_synchronize_nowait () [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.

6.90.2.5 bool 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.

6.90.2.6 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.

6.90.2.7 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.

6.90.2.8 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.

6.90.3 Member Data Documentation

6.90.3.1 DakotaString SurrLayeredModel::actualInterfacePointer [private]

string identifier for 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.

6.90.3.2 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

6.91 SurrogateDataPoint Class Reference

Simple container class encapsulating basic parameter and response data for defining a "truth" data point.

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.

6.91.1 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).

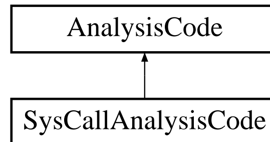
The documentation for this class was generated from the following file:

- DakotaApproximation.H

6.92 SysCallAnalysisCode Class Reference

Derived class in the AnalysisCode class hierarchy which spawns simulations using system calls.

Inheritance diagram for SysCallAnalysisCode::



Public Methods

- SysCallAnalysisCode (const ProblemDescDB &problem_db)

  constructor.

- ~SysCallAnalysisCode ()

  destructor.

- void spawn_evaluation (const bool block_flag)

  spawn a complete function evaluation.

- void spawn_input_filter (const bool block_flag)

  spawn the input filter portion of a function evaluation.

- void spawn_analysis (const int &analysis_id, const bool block_flag)

  spawn a single analysis as part of a function evaluation.

- void spawn_output_filter (const bool 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).

6.92.1 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.

6.92.2 Member Function Documentation

6.92.2.1 void SysCallAnalysisCode::spawn_evaluation (const bool *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.

6.92.2.2 void SysCallAnalysisCode::spawn_input_filter (const bool *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.

6.92.2.3 void SysCallAnalysisCode::spawn_analysis (const int & *analysis_id*, const bool *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.

6.92.2.4 void SysCallAnalysisCode::spawn_output_filter (const bool *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.

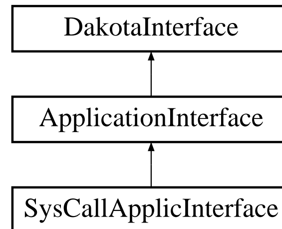
The documentation for this class was generated from the following files:

- SysCallAnalysisCode.H
- SysCallAnalysisCode.C

6.93 SysCallApplicInterface Class Reference

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

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 (DakotaPRPList &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 (DakotaPRPList &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 bool 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 (DakotaPRPList &prp_list)

  Convenience function for common code between derived_synch() & derived_synch_nowait().

- bool 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.

6.93.1 Detailed Description

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

SysCallApplicInterface uses a SysCallAnalysisCode object for performing simulation invocations.

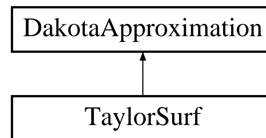
The documentation for this class was generated from the following files:

- SysCallApplicInterface.H
- SysCallApplicInterface.C

6.94 TaylorSurf Class Reference

Derived approximation class for 1st order Taylor series (local approximation).

Inheritance diagram for TaylorSurf::



Public Methods

- TaylorSurf (const ProblemDescDB &problem_db, const size_t &num_acv)

  constructor.

- ~TaylorSurf ()

  destructor.

Protected Methods

- void find_coefficients ()

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

- int required_samples ()

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

6.94.1 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)

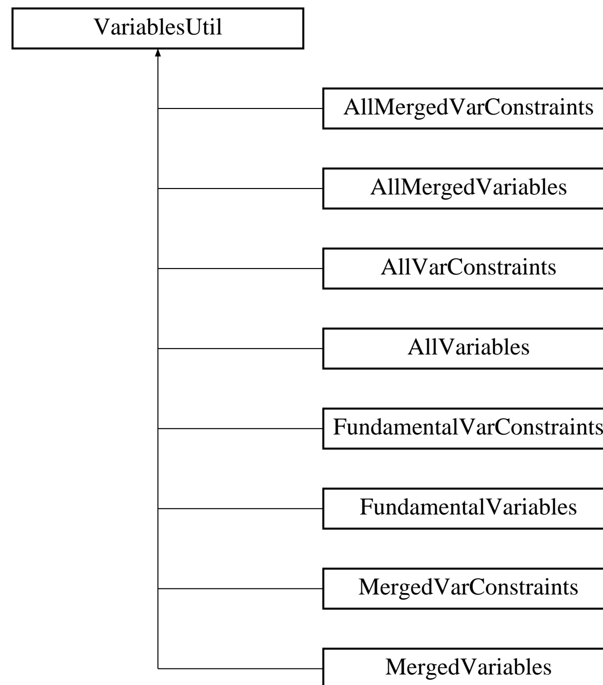
The documentation for this class was generated from the following files:

- TaylorSurf.H
- TaylorSurf.C

6.95 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.

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) const

  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) const

  combine 3 label arrays (design, uncertain, state) into a single label array (all view).

6.95.1 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

- int main (int argc, char *argv[ ])
  The main DAKOTA program.

Variables

- int write_precision = 10
  used in ostream data output functions.

7.2.1 Detailed Description

file containing the main program for DAKOTA.

7.2.2 Function Documentation

7.2.2.1 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, DakotaString identifier_type)

  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

- 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*, DakotaString *identifier_type*)

repair a restart file by removing corrupted evaluations.

Usage: "dakota_restart_util remove 0.0 dakota_old.rst dakota_new.rst"

"dakota_restart_util remove_ids 2 7 13 dakota_old.rst dakota_new.rst"

Repairs a restart file by removing corrupted evaluations. The identifier for evaluation removal can be either a double precision number (all evaluations having a matching response function value are removed) or a list of integers (all evaluations with matching evaluation ids are removed).

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

Interfacing with DAKOTA as a Library

8.1 Introduction

Some users may be interested in linking the DAKOTA toolkit into another application for use as an algorithm library. While this is not the primary use model for DAKOTA, certain facilities are in place to allow this type of integration.

As part of the normal DAKOTA build process, a `libdakota.a` is created and a copy of it is placed in `Dakota/lib`. This library contains all source files from `Dakota/src` excepting the main.C and restart_util.C main programs. This library may be linked with another application through inclusion of `-ldakota` on the link line. Library and header paths may also be specified using the -L and -I compiler options. Depending on the configuration used when building this library, other libraries for the vendor optimizers and vendor packages will also be needed to resolve DAKOTA symbols for DOT, NPSOL, OPT++, SGOPT, LHS, Epetra, etc. Copies of these libraries are also placed in `Dakota/lib`. An XML specification of library names and paths is also available in `Dakota/dependency`.

Warning:

While users are free to interface DAKOTA as a library within other software applications for their own internal use, the GNU GPL license stipulates that any application linked with DAKOTA in this way defines a "derivative work" and can only be distributed externally under the same GNU GPL open source license. Refer to `http://www.gnu.org/licenses/gpl.html` or contact the DAKOTA team for additional information.

Attention:

The use of DAKOTA as an algorithm library should be distinguished from the linking of simulations within DAKOTA using the direct application interface (see DirectFnApplicInterface). In the former, DAKOTA is providing algorithm services to another software application, and in the latter, a linked simulation is providing analysis services to DAKOTA.

The procedure for linking DAKOTA within another application is most easily explained with reference to main.C. The basic steps of executing DAKOTA include management of command line inputs and input files (ProblemDescDB::manage_inputs()), managing restart files and output streams (ParallelLibrary::manage_outputs_restart()), initializing and freeing top level parallel iterator communicators (ParallelLibrary::init_iterator_communicators() and ParallelLibrary::free_iterator_communicators), and instantiating the DakotaStrategy and running it (DakotaStrategy::run_strategy()). When using DAKOTA

as an algorithm library, these same basic operations must still be performed, although the syntax will be different from that in main.C. In particular, main.C can pass command line attributes to ProblemDescDB::manage_inputs() and ParallelLibrary::manage_outputs_restart(), whereas in an algorithm library approach, command line information will not in general be accessible.

To replace information previously obtained from the command line, overloaded forms of these functions have been developed in which the required information is passed through the parameter lists. In the case of managing restart files and output streams, the call to

```
parallel_lib.manage_outputs_restart(cmd_line_handler);
```

should be replaced with its overloaded form

```
parallel_lib.manage_outputs_restart(std_output_filename,
  std_error_filename, read_restart_filename, write_restart_filename,
  restart_evals);
```

where file names for standard output and error and restart read and write as well as the integer number of restart evaluations are passed through the parameter list rather than read from the command line of the main DAKOTA program. The definition of these attributes is performed elsewhere in the parent application (e.g., specified in the parent application input file or GUI).

With respect to modifying ProblemDescDB::manage_inputs(), the two following sections describe different approaches to populating data within DAKOTA's problem description database. It is this database from which all DAKOTA objects draw data upon instantiation.

8.2 Problem database populated through input file parsing

The simplest approach to linking an application with the DAKOTA library is to rely on DAKOTA's normal parsing system to populate DAKOTA's problem database (ProblemDescDB) through the reading of an input file. The disadvantage to this approach is the requirement for an additional input file beyond those already required by the parent application.

In this approach, the call to

```
problem_db.manage_inputs(argc, argv, cmd_line_handler);
```

should be replaced with its overloaded form

```
problem_db.manage_inputs(dakota_input_file);
```

where the file name for the DAKOTA input is passed through the parameter list rather than read from the command line of the main DAKOTA program. Again, the definition of the DAKOTA input file name is performed elsewhere in the parent application (e.g., specified in the parent application input file or GUI).

8.3 Problem database populated through external means

This approach is more involved than the previous approach, but it allows the application to publish all needed data to DAKOTA's database directly, thereby eliminating the need for the parsing of a separate

DAKOTA input file. In this case, ProblemDescDB::manage_inputs() is not called. Rather, DataStrategy, DataMethod, DataVariables, DataInterface, and DataResponses objects must be instantiated and populated with the desired problem data. These objects are then published to the problem database using ProblemDescDB::insert_node(), e.g.:

```
// instantiate the data object
DataMethod data_method;

// set the attributes within the data object
data_method.methodName = "nond_sampling";
...

// publish the data object to the ProblemDescDB
problem_db.insert_node(data_method);
```

The data objects are populated with their default values upon instantiation, so only the non-default values need to be specified. Refer to the DataStrategy, DataMethod, DataVariables, DataInterface, and DataResponses class documentation and source code for lists of attributes and their defaults.

The default strategy is `single_method`, which runs a single iterator on a single model, so it is not necessary to instantiate and publish a DataStrategy object if coordination of multiple iterators and models is not required. Rather, instantiation and insertion of a single DataMethod, DataVariables, DataInterface, and DataResponses object is sufficient for basic DAKOTA capabilities.

Once the data objects have been published to the ProblemDescDB object, a call to

```
problem_db.check_input();
```

will perform basic database error checking.

8.4 Performing an iterative study

With the ProblemDescDB object populated with problem data, the next step is to instantiate and run the strategy:

```
// instantiate the strategy
DakotaStrategy selected_strategy(problem_db);

// run the strategy
selected_strategy.run_strategy();
```

8.5 Retrieving data after a run

After executing the strategy, final results can be obtained through the use of DakotaStrategy::strategy_variable_results() and DakotaStrategy::strategy_response_results(), e.g.:

```
// retrieve the final parameter values
const DakotaVariables& vars = selected_strategy.strategy_variable_results();

// retrieve the final response values
const DakotaResponse& resp  = selected_strategy.strategy_response_results();
```

In the case of optimization, the final design is returned, and in the case of uncertainty quantification, the final statistics are returned.

8.6 Summary

To utilize the DAKOTA library within a parent software application, the basic steps of main.C and the order of invocation of these steps should be mimicked from within the parent application. Of these steps, ProblemDescDB::manage_inputs() and ParallelLibrary::manage_outputs_restart() require the modifications described herein in order to perform in an environment without direct command line access and, potentially, without file parsing.

DAKOTA's library mode is a relatively new capability and feedback from the user community for making it more useful is welcome.

Chapter 9

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.

9.1 Synchronous function evaluations

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.

9.2 Asynchronous function evaluations

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.

9.3 Analyses within each function evaluation

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

Chapter 10

Recommended Practices for DAKOTA Development

10.1 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.

10.2 Style Guidelines

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

10.2.1 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;
```

10.2.2 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
```

10.2.3 Miscellaneous

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

```
typedef double Real;
```

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

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

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

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

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

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

```
  const 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).

10.3 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.

10.4 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 1.5 2003/04/04 22:13:02 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 11

Instructions for Modifying DAKOTA's Input Specification

11.1 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`).

11.2 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.

11.3 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.

11.4 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.

11.4.1 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.

11.4.2 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 the method, variables, interface, and responses keyword handlers, a Data class object is instantiated in order to store attributes, e.g.:

```
DataMethod data_method;
```

and within the strategy keyword handler, the strategySpec data class object is used to store attributes. Each of these data class objects 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, ProblemDescDB::responsesList, and ProblemDescDB::strategySpec 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 of 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).

11.4.3 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 (*variablesIter).continuousDesignVars;
```

appears at the top of ProblemDescDB::get_drv(). Based on the identifier string, it returns the `continuousDesignVars` attribute from a DataVariables object. Since there may be multiple variables specifications, the `variablesIter` list iterator identifies which node in the 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 `variablesIter`, 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 a list of DataStrategy objects is not needed. Rather, strategySpec is the lone DataStrategy object.

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 `(*listIter).attribute` 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 (*methodIter).methodSetting;
```

A strategy specification addition would not use a `(*listIter)` syntax, but would instead look like:

```
else if (entry_name == "strategy.strategy_name.strategy_setting")
  return strategySpec.strategySetting;
```

11.5 Update Corresponding Data Classes

In this step, we extend the Data class definitions (DataStrategy, DataMethod, DataVariables, DataInterface, and/or DataResponses) to include the new attributes referenced in Update keyword handler logic blocks and Augment/update get_<data_type>() functions.

11.5.1 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 attribute naming conventions (or mimic the existing code).

11.5.2 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.

11.6 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 iterators (i.e., `methodIter`, `interfaceIter`, `variablesIter`, and `responsesIter`) 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.

11.7 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.

Index

~ANNSurf
ANNSurf, 42
~AllMergedVarConstraints
AllMergedVarConstraints, 25
~AllMergedVariables
AllMergedVariables, 28
~AllVarConstraints
AllVarConstraints, 32
~AllVariables
AllVariables, 35
~AnalysisCode
AnalysisCode, 40
~ApplicationInterface
ApplicationInterface, 44
~ApproximationInterface
ApproximationInterface, 55
~BranchBndStrategy
BranchBndStrategy, 59
~COLINApplication
COLINApplication, 61
~COLINOptimizer
COLINOptimizer, 64
~CONMINOptimizer
CONMINOptimizer, 72
~CommandLineHandler
CommandLineHandler, 67
~CommandShell
CommandShell, 68
~ConcurrentStrategy
ConcurrentStrategy, 70
~CtelRegexp
CtelRegexp, 79
~DACEIterator
DACEIterator, 81
~DOTOptimizer
DOTOptimizer, 212
~DakotaApproximation
DakotaApproximation, 88
~DakotaArray
DakotaArray, 90
~DakotaBaseVector
DakotaBaseVector, 94
~DakotaBiStream
DakotaBiStream, 100
~DakotaBoStream
DakotaBoStream, 101
~DakotaGraphics
DakotaGraphics, 104
~DakotaInterface
DakotaInterface, 111
~DakotaIterator
DakotaIterator, 118
~DakotaLeastSq
DakotaLeastSq, 120
~DakotaList
DakotaList, 122
~DakotaMatrix
DakotaMatrix, 126
~DakotaModel
DakotaModel, 136
~DakotaNonD
DakotaNonD, 139
~DakotaOptLeastSq
DakotaOptLeastSq, 147
~DakotaOptimizer
DakotaOptimizer, 143
~DakotaResponse
DakotaResponse, 150
~DakotaResponseRep
DakotaResponseRep, 154
~DakotaStrategy
DakotaStrategy, 162
~DakotaString
DakotaString, 165
~DakotaVarConstraints
DakotaVarConstraints, 172
~DakotaVariables
DakotaVariables, 178
~DakotaVector
DakotaVector, 180
~DataInterface
DataInterface, 184
~DataMethod
DataMethod, 189
~DataResponses
DataResponses, 196
~DataStrategy
DataStrategy, 199
~DataVariables
DataVariables, 203

~DirectFnApplicInterface
DirectFnApplicInterface, 208
~ForkAnalysisCode
ForkAnalysisCode, 217
~ForkApplicInterface
ForkApplicInterface, 219
~FundamentalVarConstraints
FundamentalVarConstraints, 223
~FundamentalVariables
FundamentalVariables, 227
~GetLongOpt
GetLongOpt, 232
~HermiteSurf
HermiteSurf, 236
~HierLayeredModel
HierLayeredModel, 238
~KrigApprox
KrigApprox, 242
~KrigingSurf
KrigingSurf, 250
~LayeredModel
LayeredModel, 252
~MARSSurf
MARSSurf, 257
~MergedVarConstraints
MergedVarConstraints, 259
~MergedVariables
MergedVariables, 262
~MultilevelOptStrategy
MultilevelOptStrategy, 266
~NLSSOLLeastSq
NLSSOLLeastSq, 275
~NPSOLOptimizer
NPSOLOptimizer, 294
~NestedModel
NestedModel, 269
~NonDAdvMeanValue
NonDAdvMeanValue, 278
~NonDLHSSampling
NonDLHSSampling, 285
~NonDOptStrategy
NonDOptStrategy, 287
~NonDPCESampling
NonDPCESampling, 289
~NonDSampling
NonDSampling, 291
~ParallelLibrary
ParallelLibrary, 297
~ParamResponsePair
ParamResponsePair, 309
~ParamStudy
ParamStudy, 312
~ProblemDescDB
ProblemDescDB, 316
~RespSurf
RespSurf, 321
~SGOPTApplication
SGOPTApplication, 325
~SGOPTOptimizer
SGOPTOptimizer, 330
~SNLLBase
SNLLBase, 335
~SNLLLeastSq
SNLLLeastSq, 338
~SNLLOptimizer
SNLLOptimizer, 341
~SOLBase
SOLBase, 346
~SingleMethodStrategy
SingleMethodStrategy, 331
~SingleModel
SingleModel, 333
~SurrBasedOptStrategy
SurrBasedOptStrategy, 350
~SurrLayeredModel
SurrLayeredModel, 355
~SurrogateDataPoint
SurrogateDataPoint, 360
~SysCallAnalysisCode
SysCallAnalysisCode, 362
~SysCallApplicInterface
SysCallApplicInterface, 364
~TaylorSurf
TaylorSurf, 366
~VariablesUtil
VariablesUtil, 367
~rSQPOptimizer
rSQPOptimizer, 323

A
CONMINOptimizer, 78
KrigApprox, 248
ABOBJ1
KrigApprox, 244
activate_model_auto_graphics
DakotaModel, 132
active_set_vector
DakotaResponse, 150
ParamResponsePair, 310
active_variables
DakotaModel, 130
activeSetVector
COLINApplication, 61
DakotaIterator, 115
SGOPTApplication, 325
activeSetVectorFlag
DataInterface, 186
actualInterfacePointer

ApproximationInterface, 57
SurrLayeredModel, 359
actualInterfacePtr
DataInterface, 186
actualInterfaceResponsesPtr
DataInterface, 186
actualModel
SurrLayeredModel, 359
acv
AllMergedVariables, 29
AllVariables, 36
DakotaVariables, 175
FundamentalVariables, 228
MergedVariables, 263
add_datapoint
DakotaGraphics, 105
add_point
DakotaApproximation, 87
add_point_rebuild
DakotaApproximation, 85
adv
AllMergedVariables, 29
AllVariables, 36
DakotaVariables, 175
FundamentalVariables, 228
MergedVariables, 263
all_c_variables
DakotaIterator, 114
all_continuous_lower_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 33
DakotaVarConstraints, 169
FundamentalVarConstraints, 224
MergedVarConstraints, 260
all_continuous_upper_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 33
DakotaVarConstraints, 169
FundamentalVarConstraints, 224
MergedVarConstraints, 260
all_continuous_variable_labels
AllMergedVariables, 29
AllVariables, 36
DakotaVariables, 175
FundamentalVariables, 228
MergedVariables, 263
all_continuous_variables
AllMergedVariables, 29
AllVariables, 36
DakotaVariables, 175
FundamentalVariables, 228
MergedVariables, 263
all_discrete_lower_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 33
DakotaVarConstraints, 169
FundamentalVarConstraints, 224
MergedVarConstraints, 260
all_discrete_upper_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 33
DakotaVarConstraints, 169
FundamentalVarConstraints, 224
MergedVarConstraints, 260
all_discrete_variable_labels
AllMergedVariables, 29
AllVariables, 36
DakotaVariables, 175
FundamentalVariables, 228
MergedVariables, 263
all_discrete_variables
AllMergedVariables, 29
AllVariables, 36
DakotaVariables, 175
FundamentalVariables, 228
MergedVariables, 263
all_fn_responses
DakotaIterator, 114
all_responses
DakotaIterator, 114
all_variables
DakotaIterator, 114
allContinuousLabels
AllVariables, 37
allContinuousLowerBnds
AllVarConstraints, 33
allContinuousUpperBnds
AllVarConstraints, 33
allContinuousVars
AllVariables, 37
allCVariables
DakotaIterator, 116
allDataFlag
DACEIterator, 82
NonDSampling, 292
allDiscreteLabels
AllVariables, 37
allDiscreteLowerBnds
AllVarConstraints, 34
allDiscreteUpperBnds
AllVarConstraints, 34
allDiscreteVars
AllVariables, 37
allFnResponses
DakotaIterator, 116
allHeaders
DakotaIterator, 116
allMergedLabels

AllMergedVariables, 30
allMergedLowerBnds
AllMergedVarConstraints, 27
allMergedUpperBnds
AllMergedVarConstraints, 27
AllMergedVarConstraints
~AllMergedVarConstraints, 25
all_continuous_lower_bounds, 26
all_continuous_upper_bounds, 26
all_discrete_lower_bounds, 26
all_discrete_upper_bounds, 26
allMergedLowerBnds, 27
allMergedUpperBnds, 27
AllMergedVarConstraints, 27
continuous_lower_bounds, 25
continuous_upper_bounds, 25
discrete_lower_bounds, 26
discrete_upper_bounds, 26
inactive_continuous_lower_bounds, 26
inactive_continuous_upper_bounds, 26
inactive_discrete_lower_bounds, 26
inactive_discrete_upper_bounds, 26
read, 27
write, 26
AllMergedVarConstraints, 25
AllMergedVarConstraints, 27
AllMergedVariables
~AllMergedVariables, 28
acv, 29
adv, 29
all_continuous_variable_labels, 29
all_continuous_variables, 29
all_discrete_variable_labels, 29
all_discrete_variables, 29
allMergedLabels, 30
AllMergedVariables, 28, 31
allMergedVars, 30
continuous_variable_labels, 28, 29
continuous_variables, 28
copy_rep, 30
cv, 28
discrete_variable_labels, 29
discrete_variables, 28
dv, 28
inactive_continuous_variables, 29
inactive_discrete_variables, 29
operator==, 30
read, 29, 30
read_annotated, 29
tv, 28
write, 29, 30
write_annotated, 29
AllMergedVariables, 28
AllMergedVariables, 31
allMergedVars
AllMergedVariables, 30
allocate_arrays
SOLBase, 346
allocate_workspace
CONMINOptimizer, 72
DOTOptimizer, 212
SOLBase, 346
allResponses
DakotaIterator, 116
AllVarConstraints
~AllVarConstraints, 32
all_continuous_lower_bounds, 33
all_continuous_upper_bounds, 33
all_discrete_lower_bounds, 33
all_discrete_upper_bounds, 33
allContinuousLowerBnds, 33
allContinuousUpperBnds, 33
allDiscreteLowerBnds, 34
allDiscreteUpperBnds, 34
AllVarConstraints, 34
continuous_lower_bounds, 32
continuous_upper_bounds, 32
discrete_lower_bounds, 32
discrete_upper_bounds, 32
inactive_continuous_lower_bounds, 32, 33
inactive_continuous_upper_bounds, 33
inactive_discrete_lower_bounds, 33
inactive_discrete_upper_bounds, 33
numCDV, 34
numCSV, 34
numDDV, 34
numDSV, 34
numUV, 34
read, 33
write, 33
AllVarConstraints, 32
AllVarConstraints, 34
AllVariables
~AllVariables, 35
acv, 36
adv, 36
all_continuous_variable_labels, 36
all_continuous_variables, 36
all_discrete_variable_labels, 36
all_discrete_variables, 36
allContinuousLabels, 37
allContinuousVars, 37
allDiscreteLabels, 37
allDiscreteVars, 37
AllVariables, 35, 38
continuous_variable_labels, 35, 36
continuous_variables, 35
copy_rep, 37

cv, 35
discrete_variable_labels, 36
discrete_variables, 35
dv, 35
inactive_continuous_variables, 36
inactive_discrete_variables, 36
numCDV, 37
numCSV, 37
numDDV, 37
numDSV, 37
numUV, 37
operator==, 38
read, 36, 37
read_annotated, 36
tv, 35
write, 36, 37
write_annotated, 36

AllVariables, 35
AllVariables, 38

allVariables
DakotaIterator, 116

allVarsFlag
DataMethod, 194
NonDLHSSampling, 285

ALPHAX
KrigApprox, 244

amvFlag
NonDAdvMeanValue, 281

analysis_communicator_rank
ParallelLibrary, 301

analysis_communicator_size
ParallelLibrary, 301

analysis_intra_communicator
ParallelLibrary, 301

analysis_master_flag
ParallelLibrary, 301

analysis_server_id
ParallelLibrary, 301

analysis_servers
ParallelLibrary, 301

AnalysisCode
~AnalysisCode, 40
AnalysisCode, 40
apreproFlag, 40
define_filenames, 39
fileNameKey, 41
fileSaveFlag, 40
fileTagFlag, 40
iFilterName, 40
input_filter_name, 39
modified_parameters_filename, 39
modified_results_filename, 39
modifiedParamsFileName, 40
modifiedResFileName, 40
numPrograms, 40
oFilterName, 40
output_filter_name, 39
parallelLib, 41
parametersFileName, 40
parametersFNameList, 41
program_names, 39
programNames, 40
read_results_file, 39
results_fname, 39
resultsFileName, 40
resultsFNameList, 41
suppress_output_flag, 39
suppressOutputFlag, 40
verboseFlag, 40
write_parameters_file, 39

AnalysisCode, 39

analysisComm
ApplicationInterface, 47

analysisCommRank
ApplicationInterface, 46
ParallelLibrary, 305

analysisCommSize
ApplicationInterface, 46
ParallelLibrary, 305

analysisDrivers
ApplicationInterface, 47
DataInterface, 185

analysisIntraComm
ParallelLibrary, 305

analysisMasterFlag
ParallelLibrary, 305

analysisMessagePass
ApplicationInterface, 46

analysisScheduling
ApplicationInterface, 48
DataInterface, 186

analysisServerId
ApplicationInterface, 46
ParallelLibrary, 305

analysisServers
DataInterface, 186

analysisUsage
DataInterface, 185

annObject
ANNSurf, 42

ANNSurf, 42
~ANNSurf, 42
annObject, 42
ANNSurf, 42
find_coefficients, 42
get_value, 42
required_samples, 42

ApplicationInterface

~ApplicationInterface, 44
analysisComm, 47
analysisCommRank, 46
analysisCommSize, 46
analysisDrivers, 47
analysisMessagePass, 46
analysisScheduling, 48
analysisServerId, 46
ApplicationInterface, 44
asvControlFlag, 49
asynch_local_evaluation_concurrency, 44
asynchLocalAnalysisConcurrency, 46
asynchLocalAnalysisFlag, 46
asynchLocalEvalConcurrency, 48
beforeSynchDuplicateIds, 49
beforeSynchDuplicateIndices, 49
beforeSynchDuplicateResponses, 49
beforeSynchPRPList, 50
clear_bookkeeping, 45
continuation, 48
defaultASV, 49
derived_map, 45
derived_map_asynch, 45
derived_synch, 45
derived_synch_nowait, 45
derived_synchronous_local_analysis, 45
evalAnalysisIntraComm, 47
evalCacheFlag, 49
evalComm, 47
evalCommRank, 46
evalCommSize, 46
evalDedMasterFlag, 46
evalMessagePass, 46
evalScheduling, 48
evalServerId, 46
failAction, 49
failRecoveryFnVals, 49
failRetryLimit, 49
free_communicators, 44
get_source_pair, 48
headerFlag, 49
historyDuplicateIds, 49
historyDuplicateResponses, 49
init_communicators, 44
interface_synchronization, 44
interfaceSynchronization, 49
iteratorCommRank, 46
iteratorCommSize, 46
lenPRPairMessage, 47
lenResponseMessage, 47
lenVarsASVMessage, 47
lenVarsMessage, 47
manage_failure, 44
multiProcAnalysisFlag, 47
numAnalysisDrivers, 47
numAnalysisServers, 47
numEvalServers, 48
parallelLib, 45
procsPerAnalysis, 48
restartFileFlag, 49
runningList, 50
suppressOutput, 46
worldRank, 46
worldSize, 46
ApplicationInterface, 44
asynchronous_local_evaluations, 52
asynchronous_local_evaluations_nowait, 53
duplication_detect, 52
init_serial, 50
map, 50
self_schedule_analyses, 51
self_schedule_evaluations, 52
serve_analyses_synch, 51
serve_evaluations, 51
serve_evaluations_asynch, 53
serve_evaluations_peer, 54
serve_evaluations_synch, 53
static_schedule_evaluations, 52
stop_evaluation_servers, 51
synch, 50
synch_nowait, 51
synchronous_local_evaluations, 53
apply_correction
DakotaModel, 129
LayeredModel, 252
approxBuilds
LayeredModel, 255
approxCorrectionOrder
DataInterface, 187
approxCorrectionType
DataInterface, 187
approxDaceMethodPtr
DataInterface, 187
approxGradUsageFlag
DataInterface, 187
approximateModel
SurrBasedOptStrategy, 351
approximation_coefficients
ApproximationInterface, 55
DakotaApproximation, 85
DakotaInterface, 108
DakotaModel, 129
HermiteSurf, 236
RespSurf, 321
SurrLayeredModel, 356
ApproximationInterface
~ApproximationInterface, 55
approximation_coefficients, 55

ApproximationInterface, 55
beforeSynchResponseList, 56
build_global_approximation, 55
build_local_approximation, 55
functionSurfaceCoeffs, 56
graphicsFlag, 56
map, 55
minimum_samples, 55
minSamples, 56
sampleReuse, 56
sampleReuseFile, 56
synch, 56
synch_nowait, 56
update_approximation, 55
ApproximationInterface, 55
actualInterfacePointer, 57
daceMethodPointer, 57
functionSurfaces, 57
approxInterface
SurrLayeredModel, 356
approxLowerBounds
DakotaApproximation, 87
approxRep
DakotaApproximation, 87
approxSampleReuse
DataInterface, 187
approxSampleReuseFile
DataInterface, 187
approxType
DakotaApproximation, 86
DataInterface, 186
LayeredModel, 253
approxUpperBounds
DakotaApproximation, 87
aPPSOptimizer
SGOPTOptimizer, 329
apreproFlag
AnalysisCode, 40
DakotaVariables, 177
apreproFormatFlag
DataInterface, 185
argC
BranchBndStrategy, 60
argList
ForkAnalysisCode, 217
argument_list
ForkAnalysisCode, 217
argV
BranchBndStrategy, 60
array
DakotaBaseVector, 96
assign
DataInterface, 187
DataMethod, 195
DataResponses, 198
DataStrategy, 201
DataVariables, 207
assign_rep
DakotaInterface, 111
asv_mapping
NestedModel, 270
asvControlFlag
ApplicationInterface, 49
asvList
DakotaModel, 135
asynch_compute_response
DakotaModel, 129, 130
asynch_flag
CommandShell, 68
DakotaModel, 132
asynch_local_evaluation_concurrency
ApplicationInterface, 44
DakotaInterface, 108
asynchEvalFlag
DakotaModel, 134
asynchFDFlag
DakotaModel, 134
asynchFlag
CommandShell, 68
DakotaIterator, 116
asynchLocalAnalysisConcurrency
ApplicationInterface, 46
DataInterface, 185
asynchLocalAnalysisFlag
ApplicationInterface, 46
asynchLocalEvalConcurrency
ApplicationInterface, 48
DataInterface, 185
asynchronous_local_analyses
ForkApplicInterface, 221
asynchronous_local_evaluations
ApplicationInterface, 52
asynchronous_local_evaluations_nowait
ApplicationInterface, 53
augment_bounds
SOLBase, 346
auto_correction
DakotaModel, 129
LayeredModel, 252
autoCorrection
LayeredModel, 255

B
CONMINOptimizer, 77
KrigApprox, 248
badScalingFlag
LayeredModel, 254
BaseConstructor

BaseConstructor, 58
BaseConstructor, 58
basename
GetLongOpt, 233
baseOptimizer
SGOPTOptimizer, 329
batchSize
DataMethod, 193
bcast
ParallelLibrary, 298
beforeSynchDuplicateIds
ApplicationInterface, 49
beforeSynchDuplicateIndices
ApplicationInterface, 49
beforeSynchDuplicateResponses
ApplicationInterface, 49
beforeSynchIdList
DakotaInterface, 109
beforeSynchPRPList
ApplicationInterface, 50
beforeSynchResponseList
ApproximationInterface, 56
bestObjectiveFn
DACEIterator, 82
ParamStudy, 314
bestResponses
DACEIterator, 82
DakotaOptLeastSq, 148
ParamStudy, 314
SurrBasedOptStrategy, 353
bestVariables
DACEIterator, 82
DakotaOptLeastSq, 148
ParamStudy, 314
SurrBasedOptStrategy, 353
bestViolations
DACEIterator, 82
ParamStudy, 314
betaApproxCenterGrads
LayeredModel, 254
betaApproxCenterVals
LayeredModel, 254
betaCenterPt
LayeredModel, 254
betaFns
LayeredModel, 254
betaGrads
LayeredModel, 254
betaHat
KrigApprox, 245
bigIntBoundSize
DakotaOptLeastSq, 147
bigRealBoundSize
DakotaOptLeastSq, 147
boundConstraintFlag
DakotaOptLeastSq, 148
boundsArraySize
SOLBase, 347
branchBndNumSamplesNode
DataStrategy, 200
branchBndNumSamplesRoot
DataStrategy, 200
BranchBndStrategy
~BranchBndStrategy, 59
argC, 60
argV, 60
BranchBndStrategy, 59
numIteratorServers, 59
numNodeSamples, 59
numRootSamples, 59
picoComm, 59
picoCommRank, 59
picoCommSize, 60
picoListOfIntegers, 60
picoLowerBnds, 60
picoUpperBnds, 60
run_strategy, 59
selectedIterator, 59
userDefinedModel, 59
BranchBndStrategy, 59
build
DakotaApproximation, 85
build_approximation
DakotaModel, 128
HierLayeredModel, 238
SurrLayeredModel, 358
build_global_approximation
ApproximationInterface, 55
DakotaInterface, 108
build_label
ProblemDescDB, 318
build_labels
ProblemDescDB, 318
build_labels_partial
ProblemDescDB, 319
build_local_approximation
ApproximationInterface, 55
DakotaInterface, 108

C
CONMINOptimizer, 77
KrigApprox, 248
cantilever
DirectFnApplicInterface, 210
centered_loop
ParamStudy, 313
centeringParam
DataMethod, 192

centralPath
DataMethod, 191
chaosCoeffs
HermiteSurf, 237
chaosSamples
HermiteSurf, 237
check_error
NonDSampling, 292
check_input
ProblemDescDB, 316
check_status
ForkAnalysisCode, 218
check_submodel_compatibility
LayeredModel, 252
check_usage
CommandLineHandler, 67
cholCorrMatrix
NonDAdvMeanValue, 280
cLambda
SOLBase, 347
clear_bookkeeping
ApplicationInterface, 45
clearErrors
CtelRegexp, 79
close
DakotaGraphics, 104
close_streams
ParallelLibrary, 308
coeffArray
NonDPCESampling, 289
COLINApplication, 61
~COLINApplication, 61
activeSetVector, 61
COLINApplication, 61
dakota_asynch_flag, 62
dakota_vars, 62
dakotaCompletionList, 61
dakotaModelAsynchFlag, 61
dakotaResponseList, 61
DoEval, 62
map_response, 63
multiobjModifyPtr, 62
next_eval, 62
num_integer_params, 62
num_real_params, 62
numNonlinCons, 62
numObjFns, 61
synchronize, 62
userDefinedModel, 61
COLINOptimizer, 64
~COLINOptimizer, 64
COLINOptimizer, 64
find_optimum, 65
get_min_point, 64
optimizer, 64
problem, 64
rng, 65
set_initial_point, 64
set_method_options, 64
set_rng, 64
set_standard_method_options, 65
ColinPoint
ivec, 66
rvec, 66
ColinPoint, 66
command_usage
SysCallAnalysisCode, 362
CommandLineHandler
~CommandLineHandler, 67
check_usage, 67
CommandLineHandler, 67
read_restart_evals, 67
CommandLineHandler, 67
CommandShell
~CommandShell, 68
asynch_flag, 68
asynchFlag, 68
CommandShell, 68
operator<<, 68
suppress_output_flag, 68
suppressOutputFlag, 68
unixCommand, 68
CommandShell, 68
flush, 69
commandUsage
SysCallAnalysisCode, 362
compile
CtelRegexp, 79
completionList
DakotaInterface, 109
NestedModel, 271
compute_correction
DakotaModel, 129
LayeredModel, 254
compute_penalty_function
SurrBasedOptStrategy, 353
compute_response
DakotaModel, 129
compute_statistics
NonDSampling, 291
compute_vector_steps
ParamStudy, 312
concatenate_restart
restart_util.C, 372
concurrentParameterSets
DataStrategy, 201
concurrentRandomJobs
DataStrategy, 201

concurrentSeed
  DataStrategy, 201
ConcurrentStrategy
  ~ConcurrentStrategy, 70
  ConcurrentStrategy, 70
  iteratorServerId, 71
  multiStartFlag, 70
  numIteratorJobs, 70
  numIteratorServers, 70
  parameterSets, 70
  run_strategy, 70
  selectedIterator, 70
  strategyDedicatedMasterFlag, 71
  userDefinedModel, 70
ConcurrentStrategy, 70
conminDesVars
  CONMINOptimizer, 74
conminInfo
  CONMINOptimizer, 75
  KrigApprox, 243
conminLowerBnds
  CONMINOptimizer, 74
CONMINOptimizer, 72
  ~CONMINOptimizer, 72
  A, 78
  allocate_workspace, 72
  B, 77
  C, 77
  conminDesVars, 74
  conminInfo, 75
  conminLowerBnds, 74
  CONMINOptimizer, 72
  conminUpperBnds, 74
  constraintMappingIndices, 76
  constraintMappingMultipliers, 76
  constraintMappingOffsets, 76
  CT, 77
  CTL, 74
  CTLMIN, 74
  CTMIN, 73
  DABFUN, 74
  DELFUN, 74
  DF, 77
  FDCH, 73
  FDCHM, 73
  find_optimum, 72
  G1, 77
  G2, 77
  IC, 78
  IPRINT, 73
  ISC, 78
  ITMAX, 73
  localConstraintValues, 75
  MS1, 77
  N1, 76
  N2, 76
  N3, 76
  N4, 76
  N5, 76
  NFDG, 73
  optimizationType, 75
  printControl, 75
  S, 77
  SCAL, 77
conminSingleArray
  KrigApprox, 242
conminThetaLowerBnds
  KrigApprox, 244
conminThetaUpperBnds
  KrigApprox, 244
conminThetaVars
  KrigApprox, 244
conminUpperBnds
  CONMINOptimizer, 74
constantASVFlag
  SNLLBase, 336
constraint0_evaluator
  SNLLOptimizer, 344
constraint1_evaluator
  SNLLOptimizer, 344
constraint2_evaluator
  SNLLOptimizer, 344
constraint2_evaluator_gn
  SNLLLeastSq, 338
constraint_eval
  SOLBase, 347
constraintJacMatrixF77
  SOLBase, 348
constraintMappingIndices
  CONMINOptimizer, 76
  DOTOptimizer, 215
constraintMappingMultipliers
  CONMINOptimizer, 76
  DOTOptimizer, 215
constraintMappingOffsets
  CONMINOptimizer, 76
  DOTOptimizer, 215
constraintState
  SOLBase, 347
constraintTol
  DakotaOptLeastSq, 147
  SurrBasedOptStrategy, 351
constraintTolerance
  DataMethod, 190
constraintVector
  KrigApprox, 246
constrCoeffs
  NestedModel, 271

contains
DakotaList, 124
DakotaString, 166
continuation
ApplicationInterface, 48
continuous_lower_bounds
AllMergedVarConstraints, 25
AllVarConstraints, 32
DakotaModel, 131
DakotaVarConstraints, 168
FundamentalVarConstraints, 223
MergedVarConstraints, 259
continuous_upper_bounds
AllMergedVarConstraints, 25
AllVarConstraints, 32
DakotaModel, 131
DakotaVarConstraints, 168
FundamentalVarConstraints, 223
MergedVarConstraints, 259
continuous_variable_labels
AllMergedVariables, 28, 29
AllVariables, 35, 36
DakotaModel, 130
DakotaVariables, 175
FundamentalVariables, 227, 228
MergedVariables, 262, 263
continuous_variables
AllMergedVariables, 28
AllVariables, 35
DakotaModel, 130
DakotaVariables, 174
FundamentalVariables, 227
MergedVariables, 262
continuousDesignLabels
DataVariables, 205
FundamentalVariables, 229
continuousDesignLowerBnds
DataVariables, 204
FundamentalVarConstraints, 224
continuousDesignUpperBnds
DataVariables, 204
FundamentalVarConstraints, 225
continuousDesignVars
DataVariables, 204
FundamentalVariables, 229
continuousStateLabels
DataVariables, 207
FundamentalVariables, 230
continuousStateLowerBnds
DataVariables, 207
FundamentalVarConstraints, 225
continuousStateUpperBnds
DataVariables, 207
FundamentalVarConstraints, 225
continuousStateVars
DataVariables, 206
FundamentalVariables, 229
continuousVars
SurrogateDataPoint, 360
contractAfterFail
DataMethod, 193
contractFactor
DataMethod, 192
convergenceFlag
SurrBasedOptStrategy, 351
convergenceTol
DakotaOptLeastSq, 147
SurrBasedOptStrategy, 351
convergenceTolerance
DataMethod, 190
copy
DakotaResponse, 151
DakotaVariables, 179
SGOPTApplication, 325
copy_con_grad
SNLLBase, 336
copy_con_hess
SNLLBase, 336
copy_con_vals
SNLLBase, 336
copy_rep
AllMergedVariables, 30
AllVariables, 37
DakotaVariables, 177
FundamentalVariables, 229
MergedVariables, 264
copy_results
DakotaResponse, 152
DakotaResponseRep, 155
correctedRespLevel
NonDAdvMeanValue, 284
correctedResponseArray
LayeredModel, 252
correctedResponseList
LayeredModel, 253
correctionComputed
LayeredModel, 254
correctionFlag
SurrBasedOptStrategy, 352
correctionOrder
LayeredModel, 253
correctionType
LayeredModel, 253
correlationFlag
DakotaNonD, 141
correlationMatrix
KrigApprox, 246
correlationVector

KrigingSurf, 250
create_plots_2d
DakotaGraphics, 105
create_tabular_datastream
DakotaGraphics, 105
crossoverRate
DataMethod, 192
crossoverType
DataMethod, 193
CT
CONMINOptimizer, 77
KrigApprox, 247
CtelRegexp
~CtelRegexp, 79
clearErrors, 79
compile, 79
CtelRegexp, 79, 80
getRe, 79
getStatus, 79
getStatusMsg, 79
match, 79
operator=, 80
r, 80
split, 79
status, 80
statusMsg, 80
strPattern, 80
CtelRegexp, 79
CTL
CONMINOptimizer, 74
KrigApprox, 243
CTLMIN
CONMINOptimizer, 74
KrigApprox, 243
CTMIN
CONMINOptimizer, 73
KrigApprox, 243
current_response
DakotaModel, 132
current_variables
DakotaModel, 132
currentPoints
DakotaApproximation, 86
currentResponse
DakotaModel, 133
currentVariables
DakotaModel, 133
cv
AllMergedVariables, 28
AllVariables, 35
DakotaModel, 130
DakotaVariables, 174
FundamentalVariables, 227
MergedVariables, 262
cyl_head
DirectFnApplicInterface, 210

DABFUN
CONMINOptimizer, 74
KrigApprox, 243
daceCenterPtFlag
SurrBasedOptStrategy, 352
DACEIterator, 81
~DACEIterator, 81
allDataFlag, 82
bestObjectiveFn, 82
bestResponses, 82
bestVariables, 82
bestViolations, 82
DACEIterator, 83
daceMethod, 82
iterator_response_results, 81
iterator_variable_results, 81
multiObjWeights, 83
nonlinearEqTargets, 83
nonlinearIneqLowerBnds, 83
nonlinearIneqUpperBnds, 83
numDACERuns, 82
numNonlinearEqConstraints, 83
numNonlinearIneqConstraints, 83
numObjectiveFunctions, 82
numSamples, 82
numSymbols, 82
originalSeed, 82
print_iterator_results, 81
randomSeed, 82
resolve_samples_symbols, 84
run_iterator, 83
sampling_reset, 81
sampling_scheme, 81
update_best, 81
varyPattern, 82
daceIterator
SurrLayeredModel, 357
daceMethod
DACEIterator, 82
DataMethod, 194
daceMethodPointer
ApproximationInterface, 57
SurrLayeredModel, 357
dakota_asynch_flag
COLINApplication, 62
SGOPTApplication, 326
dakota_vars
COLINApplication, 62
DakotaApproximation
add_point, 87
add_point_rebuild, 85

- approximation_coefficients, 85
- approxLowerBounds, 87
- approxRep, 87
- approxType, 86
- approxUpperBounds, 87
- build, 85
- currentPoints, 86
- DakotaApproximation, 87, 88
- draw_surface, 86
- find_coefficients, 86
- get_gradient, 85
- get_value, 85
- gradientFlag, 86
- gradVector, 86
- num_variables, 86
- numCurrentPoints, 86
- numSamples, 86
- numVars, 86
- referenceCount, 87
- required_samples, 85
- set_bounds, 86
- verboseFlag, 86

DakotaApproximation, 85
- ~DakotaApproximation, 88
- DakotaApproximation, 87, 88
- get_approx, 88
- operator=, 88

DakotaArray
- ~DakotaArray, 90
- DakotaArray, 90, 91
- length, 91
- operator=, 90
- print, 91
- read, 91
- reshape, 91

DakotaArray, 90
- DakotaArray, 91
- data, 92
- operator T ∗, 92
- operator(), 92
- operator=, 92
- operator[], 92
- testClass, 93

DakotaBaseVector
- ~DakotaBaseVector, 94
- DakotaBaseVector, 94, 95
- operator=, 94

DakotaBaseVector, 94
- array, 96
- DakotaBaseVector, 95
- data, 96
- length, 96
- operator(), 96
- operator[], 95, 96
- reshape, 96

DakotaBiStream
- DakotaBiStream, 98, 99
- inBuf, 99
- operator>>, 98, 99
- xdrInBuf, 99

DakotaBiStream, 98
- ~DakotaBiStream, 100
- DakotaBiStream, 99
- operator>>, 100

DakotaBoStream
- ~DakotaBoStream, 101
- DakotaBoStream, 101–103
- operator<<, 101, 102
- outBuf, 102
- xdrOutBuf, 102

DakotaBoStream, 101
- DakotaBoStream, 102, 103
- operator<<, 103
- testClass, 103

dakotaCompletionList
- COLINApplication, 61
- SGOPTApplication, 326

DakotaGraphics
- ~DakotaGraphics, 104
- close, 104
- DakotaGraphics, 104
- graphics2D, 104
- graphicsCntr, 104
- tabularDataFlag, 104
- tabularDataFStream, 105
- win2dOn, 104
- win3dOn, 104

DakotaGraphics, 104
- add_datapoint, 105
- create_plots_2d, 105
- create_tabular_datastream, 105
- show_data_3d, 105

DakotaInterface
- approximation_coefficients, 108
- asynch_local_evaluation_concurrency, 108
- beforeSynchIdList, 109
- build_global_approximation, 108
- build_local_approximation, 108
- completionList, 109
- DakotaInterface, 110, 111
- debugFlag, 110
- fnEvalId, 109
- free_communicators, 108
- init_communicators, 108
- init_serial, 108
- interface_synchronization, 108
- interface_type, 108
- interfaceRep, 110

interfaceType, 109
iterator_dedicated_master_flag, 109
iteratorDedMasterFlag, 109
map, 107
minimum_samples, 108
multi_proc_eval_flag, 109
multiProcEvalFlag, 109
new_eval_counter, 108
newFnEvalId, 109
quietFlag, 110
referenceCount, 110
serve_evaluations, 107
silentFlag, 109
stop_evaluation_servers, 107
synch, 107
synch_nowait, 107
synch_nowait_completions, 108
total_eval_counter, 108
update_approximation, 108
verboseFlag, 110

DakotaInterface, 107
- ~DakotaInterface, 111
- assign_rep, 111
- DakotaInterface, 110, 111
- get_interface, 111
- operator=, 111
- rawResponseArray, 112
- rawResponseList, 112

DakotaIterator
- activeSetVector, 115
- all_c_variables, 114
- all_fn_responses, 114
- all_responses, 114
- all_variables, 114
- allCVariables, 116
- allFnResponses, 116
- allHeaders, 116
- allResponses, 116
- allVariables, 116
- asynchFlag, 116
- DakotaIterator, 117, 118
- debugOutput, 116
- finiteDiffStepSize, 116
- finiteDiffType, 115
- gradientType, 115
- hessianType, 115
- is_null, 114
- iterator_response_results, 113
- iterator_variable_results, 113
- iteratorRep, 117
- maxConcurrency, 115
- maxFunctionEvals, 115
- maximum_concurrency, 114
- maxIterations, 115
- method_name, 114
- methodName, 115
- methodSource, 116
- mixedGradAnalyticIds, 116
- mixedGradNumericalIds, 116
- multi_objective_weights, 114
- numContinuousVars, 115
- numDiscreteVars, 115
- numFunctions, 115
- numVars, 115
- print_iterator_results, 113
- probDescDB, 115
- quietOutput, 116
- referenceCount, 117
- sampling_reset, 114
- sampling_scheme, 114
- silentOutput, 116
- staticModel, 116
- update_best, 114
- user_defined_model, 114
- userDefinedModel, 115
- verboseOutput, 116

DakotaIterator, 113
- ~DakotaIterator, 118
- DakotaIterator, 117, 118
- evaluate_parameter_sets, 118
- get_iterator, 119
- operator=, 118
- populate_gradient_vars, 119
- run_iterator, 118

DakotaLeastSq
- ~DakotaLeastSq, 120
- DakotaLeastSq, 120, 121
- minimize_residuals, 120
- numLeastSqTerms, 120
- staticNumLSqTerms, 121

DakotaLeastSq, 120
- DakotaLeastSq, 121
- print_iterator_results, 121
- run_iterator, 121

DakotaList
- ~DakotaList, 122
- DakotaList, 122
- entries, 122
- isEmpty, 123
- operator=, 122
- print, 122
- read, 122

DakotaList, 122
- contains, 124
- find, 124
- get, 123
- index, 124, 125
- insert, 124

occurrencesOf, 125
operator[], 125
remove, 124
removeAt, 124
sort, 124
testClass, 123
DakotaMatrix
~DakotaMatrix, 126
DakotaMatrix, 126
num_columns, 126
num_rows, 126
print, 126
read, 126
reshape_2d, 126
DakotaMatrix, 126
operator=, 127
testClass, 127
DakotaModel
activate_model_auto_graphics, 132
active_variables, 130
apply_correction, 129
approximation_coefficients, 129
asvList, 135
asynch_compute_response, 129, 130
asynch_flag, 132
asynchEvalFlag, 134
asynchFDFlag, 134
auto_correction, 129
build_approximation, 128
compute_correction, 129
compute_response, 129
continuous_lower_bounds, 131
continuous_upper_bounds, 131
continuous_variable_labels, 130
continuous_variables, 130
current_response, 132
current_variables, 132
currentResponse, 133
currentVariables, 133
cv, 130
DakotaModel, 136
dbFnsList, 135
dbResponseList, 135
deltaList, 135
derived_asynch_compute_response, 133
derived_compute_response, 133
derived_init_communicators, 133
derived_master_overload, 129
derived_synchronize, 133
derived_synchronize_nowait, 133
discrete_lower_bounds, 131
discrete_upper_bounds, 131
discrete_variable_labels, 130
discrete_variables, 130
dv, 130
finiteDiffSS, 135
free_communicators, 129
gradient_concurrency, 132
gradient_method, 132
gradType, 135
idAnalytic, 135
inactive_continuous_lower_bounds, 131
inactive_continuous_upper_bounds, 131
inactive_continuous_variables, 131
inactive_discrete_lower_bounds, 131
inactive_discrete_upper_bounds, 131
inactive_discrete_variables, 131
initialMapList, 135
intervalType, 135
is_null, 132
linear_eq_constraint_coeffs, 132
linear_eq_constraint_targets, 132
linear_ineq_constraint_coeffs, 131
linear_ineq_constraint_lower_bounds, 132
linear_ineq_constraint_upper_bounds, 132
maximum_concurrency, 128
merged_integer_list, 132
message_lengths, 132
messageLengths, 134
methodSrc, 135
model_type, 132
modelAutoGraphicsFlag, 134
modelRep, 134
modelType, 134
new_eval_counter, 129
num_functions, 130
num_linear_eq_constraints, 131
num_linear_ineq_constraints, 131
numFns, 133
numGradVars, 133
numMapsList, 135
parallelLib, 134
prob_desc_db, 132
probDescDB, 134
quietFlag, 135
referenceCount, 134
responseArray, 135
responseList, 135
serve, 129
silentFlag, 135
stop_servers, 129
subordinate_iterator, 128
subordinate_model, 128
synchronize, 130
synchronize_nowait, 130
synchronize_nowait_completions, 129
total_eval_counter, 129
tv, 130

update_approximation, 128
userDefinedVarConstraints, 133
varsList, 135
DakotaModel, 128
~DakotaModel, 136
DakotaModel, 136
fd_gradients, 137
get_model, 137
init_communicators, 137
local_eval_synchronization, 137
manage_asv, 138
operator=, 137
synchronize_fd_gradients, 138
update_response, 138
dakotaModelAsynchFlag
COLINApplication, 61
SGOPTApplication, 325
DakotaNonD
~DakotaNonD, 139
correlationFlag, 141
DakotaNonD, 139
finalStatistics, 141
histogramBinPairs, 140
histogramPointPairs, 140
iterator_response_results, 139
lognormalDistLowerBnds, 140
lognormalDistUpperBnds, 140
lognormalErrFacts, 140
lognormalMeans, 140
lognormalStdDevs, 140
loguniformDistLowerBnds, 140
loguniformDistUpperBnds, 140
mean95CIDeltas, 141
meanStats, 141
normalDistLowerBnds, 140
normalDistUpperBnds, 140
normalMeans, 139
normalStdDevs, 139
numHistogramVars, 141
numLognormalVars, 141
numLoguniformVars, 141
numNormalVars, 140
numResponseFunctions, 141
numUncertainVars, 141
numUniformVars, 141
numWeibullVars, 141
probMoreThanThresh, 141
quantify_uncertainty, 139
respThresh, 141
run_iterator, 139
stdDevStats, 141
uncertainCorrelations, 140
uniformDistLowerBnds, 140
uniformDistUpperBnds, 140
weibullAlphas, 140
weibullBetas, 140
DakotaNonD, 139
DakotaOptimizer
~DakotaOptimizer, 143
DakotaOptimizer, 143, 144
find_optimum, 143
multi_objective_weights, 143
multiObjWeights, 144
numObjectiveFunctions, 144
staticMultiObjWeights, 144
staticNumObjFns, 144
DakotaOptimizer, 143
DakotaOptimizer, 144
multi_objective_modify, 145
print_iterator_results, 144
run_iterator, 144
DakotaOptLeastSq
~DakotaOptLeastSq, 147
bestResponses, 148
bestVariables, 148
bigIntBoundSize, 147
bigRealBoundSize, 147
boundConstraintFlag, 148
constraintTol, 147
convergenceTol, 147
DakotaOptLeastSq, 146, 149
iterator_response_results, 146
iterator_variable_results, 146
linearEqConstraintCoeffs, 148
linearEqTargets, 148
linearIneqConstraintCoeffs, 147
linearIneqLowerBnds, 147
linearIneqUpperBnds, 148
nonlinearEqTargets, 147
nonlinearIneqLowerBnds, 147
nonlinearIneqUpperBnds, 147
numConstraints, 147
numLinearConstraints, 148
numLinearEqConstraints, 148
numLinearIneqConstraints, 147
numNonlinearConstraints, 147
numNonlinearEqConstraints, 147
numNonlinearIneqConstraints, 147
speculativeFlag, 148
staticNumContinuousVars, 148
staticNumNonlinearConstraints, 148
vendorNumericalGradFlag, 148
DakotaOptLeastSq, 146
DakotaOptLeastSq, 149
DakotaResponse
~DakotaResponse, 150
active_set_vector, 150
copy, 151

copy_results, 152
DakotaResponse, 150, 153
DakotaResponseRep, 156
data_size, 152
fn_tags, 150
function_gradients, 151
function_hessians, 151
function_values, 150, 151
interface_id, 150
num_functions, 150
operator
=, 152
operator=, 150
operator==, 152
overlay, 152
purge_inactive, 152
read, 151
read_annotated, 151
read_data, 152
read_tabular, 151
reset, 152
responseRep, 152
write, 151
write_annotated, 151
write_data, 152
write_tabular, 151
DakotaResponse, 150
DakotaResponse, 153
dakotaResponseList
COLINApplication, 61
SGOPTApplication, 325
DakotaResponseRep
~DakotaResponseRep, 154
copy_results, 155
DakotaResponse, 156
DakotaResponseRep, 154, 156
data_size, 155
fnTags, 155
functionGradients, 155
functionHessians, 155
functionValues, 155
interfaceId, 155
operator==, 156
overlay, 155
purge_inactive, 155
read_data, 155
referenceCount, 155
reset, 155
responseASV, 155
write_data, 155
DakotaResponseRep, 154
DakotaResponseRep, 156
read, 156–158
read_annotated, 157
read_tabular, 157
write, 157, 158
write_annotated, 157
write_tabular, 157
DakotaStrategy
DakotaStrategy, 161, 162
graphicsFlag, 161
iterator_communicator, 159
iterator_communicator_size, 160
iteratorComm, 160
iteratorCommRank, 160
iteratorCommSize, 160
mpirunFlag, 161
parallelLib, 160
probDescDB, 160
referenceCount, 161
run_strategy, 159
strategy_response_results, 159
strategy_variable_results, 159
strategyName, 160
strategyRep, 161
tabularDataFile, 161
tabularDataFlag, 161
world_rank, 159
worldRank, 160
worldSize, 160
DakotaStrategy, 159
~DakotaStrategy, 162
DakotaStrategy, 161, 162
free_communicators, 163
get_strategy, 163
init_communicators, 163
initialize_graphics, 163
operator=, 162
prob_desc_db, 164
run_iterator, 162
run_iterator_repartition, 163
DakotaString
~DakotaString, 165
DakotaString, 165
isNull, 165
operator=, 165
toLower, 165
toUpper, 165
DakotaString, 165
contains, 166
data, 166
lower, 166
operator const char *, 166
testClass, 166
upper, 166
DakotaVarConstraints
all_continuous_lower_bounds, 169
all_continuous_upper_bounds, 169

all_discrete_lower_bounds, 169
all_discrete_upper_bounds, 169
continuous_lower_bounds, 168
continuous_upper_bounds, 168
DakotaVarConstraints, 172
discrete_lower_bounds, 168
discrete_upper_bounds, 169
discreteFlag, 170
emptyIntVector, 171
emptyRealVector, 171
inactive_continuous_lower_bounds, 169
inactive_continuous_upper_bounds, 169
inactive_discrete_lower_bounds, 169
inactive_discrete_upper_bounds, 169
linear_eq_constraint_coeffs, 170
linear_eq_constraint_targets, 170
linear_ineq_constraint_coeffs, 170
linear_ineq_constraint_lower_bounds, 170
linear_ineq_constraint_upper_bounds, 170
linearEqConstraintCoeffs, 171
linearEqConstraintTargets, 171
linearIneqConstraintCoeffs, 170
linearIneqConstraintLowerBnds, 171
linearIneqConstraintUpperBnds, 171
num_active_variables, 170
num_linear_eq_constraints, 170
num_linear_ineq_constraints, 169
numLinearEqConstraints, 170
numLinearIneqConstraints, 170
read, 169
referenceCount, 171
varConstraintsRep, 171
variablesType, 170
write, 169

DakotaVarConstraints, 168
~DakotaVarConstraints, 172
DakotaVarConstraints, 172
get_var_constraints, 173
manage_linear_constraints, 173
operator=, 172

DakotaVariables
acv, 175
adv, 175
all_continuous_variable_labels, 175
all_continuous_variables, 175
all_discrete_variable_labels, 175
all_discrete_variables, 175
aprepro Flag, 177
continuous_variable_labels, 175
continuous_variables, 174
copy_rep, 177
cv, 174
DakotaVariables, 178
discrete_variable_labels, 175
discrete_variables, 175
dv, 174
emptyIntVector, 177
emptyRealVector, 177
emptyStringArray, 177
inactive_continuous_variables, 175
inactive_discrete_variables, 175
merged_integer_list, 176
mergedIntegerList, 176
operator
=, 177
operator==, 177
read, 175, 176
read_annotated, 176
referenceCount, 177
tv, 174
variables_type, 176
variablesRep, 177
variablesType, 176
write, 176
write_annotated, 176
write_tabular, 176

DakotaVariables, 174
~DakotaVariables, 178
copy, 179
DakotaVariables, 178
get_variables, 179
operator=, 179

DakotaVector
~DakotaVector, 180
DakotaVector, 180, 182
operator T *, 180
operator=, 180
print, 181, 182
print_annotated, 181
print_aprepro, 181
print_partial, 181
print_partial_aprepro, 181
read, 180, 181
read_annotated, 181
read_partial, 181
read_tabular, 181

DakotaVector, 180
DakotaVector, 182
operator=, 182
testClass, 182

data
DakotaArray, 92
DakotaBaseVector, 96
DakotaString, 166

data_size
DakotaResponse, 152
DakotaResponseRep, 155

DataInterface

~DataInterface, 184
activeSetVectorFlag, 186
actualInterfacePtr, 186
actualInterfaceResponsesPtr, 186
analysisDrivers, 185
analysisScheduling, 186
analysisServers, 186
analysisUsage, 185
approxCorrectionOrder, 187
approxCorrectionType, 187
approxDaceMethodPtr, 187
approxGradUsageFlag, 187
approxSampleReuse, 187
approxSampleReuseFile, 187
approxType, 186
apreproFormatFlag, 185
assign, 187
asynchLocalAnalysisConcurrency, 185
asynchLocalEvalConcurrency, 185
DataInterface, 184
evalCacheFlag, 186
evalScheduling, 186
evalServers, 186
failAction, 186
fileSaveFlag, 185
fileTagFlag, 185
gridHostNames, 185
gridProcsPerHost, 185
highFidelityInterfacePtr, 187
idInterface, 184
inputFilter, 184
interfaceSynchronization, 185
interfaceType, 184
krigingCorrelations, 187
lowFidelityInterfacePtr, 187
modelCenterFile, 185
operator=, 184
operator==, 184
outputFilter, 184
parametersFile, 185
polynomialOrder, 187
procsPerAnalysis, 185
read, 184
recoveryFnVals, 186
restartFileFlag, 186
resultsFile, 185
retryLimit, 186
write, 184
DataInterface, 184
DataMethod
~DataMethod, 189
allVarsFlag, 194
assign, 195
batchSize, 193
centeringParam, 192
centralPath, 191
constraintTolerance, 190
contractAfterFail, 193
contractFactor, 192
convergenceTolerance, 190
crossoverRate, 192
crossoverType, 193
daceMethod, 194
DataMethod, 189
deltasPerVariable, 195
expandAfterSuccess, 193
expansionFlag, 193
expansionOrder, 194
expansionTerms, 194
exploratoryMoves, 193
finalPoint, 194
fixedSeedFlag, 194
functionPrecision, 191
gradientTolerance, 191
idMethod, 189
initDelta, 192
interfacePointer, 189
linearEqConstraintCoeffs, 191
linearEqTargets, 191
linearIneqConstraintCoeffs, 191
linearIneqLowerBnds, 191
linearIneqUpperBnds, 191
lineSearchTolerance, 191
listOfPoints, 195
maxCPUTime, 192
maxFunctionEvaluations, 190
maxIterations, 190
maxStep, 191
meritFn, 191
methodName, 189
methodOutput, 190
minMaxType, 191
modelType, 190
mutationDimRate, 192
mutationMinScale, 192
mutationPopRate, 192
mutationRange, 193
mutationScale, 192
mutationType, 193
newSolnsGenerated, 192
nonAdaptiveFlag, 193
numberRetained, 192
numPartitions, 193
numSamples, 194
numSteps, 195
numSymbols, 194
operator=, 189
operator==, 189

optionalInterfaceResponsesPointer, 190
paramStudyType, 194
patternBasis, 193
percentDelta, 195
populationSize, 192
primaryCoeffs, 190
probabilityLevels, 194
randomizeOrderFlag, 193
randomSeed, 194
read, 189
reliabilityMethod, 194
replacementType, 193
responseLevels, 194
responsesPointer, 190
responseThresholds, 194
sampleType, 194
searchMethod, 191
searchSchemeSize, 192
secondaryCoeffs, 190
selectionPressure, 193
solnAccuracy, 192
speculativeFlag, 190
stepLength, 195
stepLenToBoundary, 191
stepVector, 194
subMethodPointer, 190
threshDelta, 192
totalPatternSize, 193
variablesPointer, 189
varPartitions, 193
verifyLevel, 191
write, 189
DataMethod, 189
DataResponses
~DataResponses, 196
assign, 198
DataResponses, 196
fdStepSize, 197
gradientType, 197
hessianType, 197
idAnalytic, 197
idNumerical, 197
idResponses, 197
intervalType, 197
methodSource, 197
multiObjectiveWeights, 197
nonlinearEqTargets, 197
nonlinearIneqLowerBnds, 197
nonlinearIneqUpperBnds, 197
numLeastSqTerms, 196
numNonlinearEqConstraints, 196
numNonlinearIneqConstraints, 196
numObjectiveFunctions, 196
numResponseFunctions, 197
operator=, 196
operator==, 196
read, 196
responseLabels, 198
write, 196
DataResponses, 196
DataStrategy
~DataStrategy, 199
assign, 201
branchBndNumSamplesNode, 200
branchBndNumSamplesRoot, 200
concurrentParameterSets, 201
concurrentRandomJobs, 201
concurrentSeed, 201
DataStrategy, 199
graphicsFlag, 199
iteratorScheduling, 200
iteratorServers, 199
methodPointer, 200
multilevelGlobalMethodPointer, 200
multilevelLocalMethodPointer, 200
multilevelLSProb, 200
multilevelMethodList, 200
multilevelProgThresh, 200
multilevelType, 200
operator=, 199
read, 199
strategyType, 199
surrBasedOptConvTol, 200
surrBasedOptMaxIterations, 200
surrBasedOptSoftConvLimit, 200
surrBasedOptTRContract, 201
surrBasedOptTRContractTrigger, 201
surrBasedOptTRExpand, 201
surrBasedOptTRExpandTrigger, 201
surrBasedOptTRInitSize, 201
surrBasedOptTRMinSize, 201
tabularDataFile, 199
tabularDataFlag, 199
write, 199
DataStrategy, 199
DataVariables
~DataVariables, 203
assign, 207
continuousDesignLabels, 205
continuousDesignLowerBnds, 204
continuousDesignUpperBnds, 204
continuousDesignVars, 204
continuousStateLabels, 207
continuousStateLowerBnds, 207
continuousStateUpperBnds, 207
continuousStateVars, 206
DataVariables, 203
design, 203

discreteDesignLabels, 205
discreteDesignLowerBnds, 204
discreteDesignUpperBnds, 205
discreteDesignVars, 204
discreteStateLabels, 207
discreteStateLowerBnds, 207
discreteStateUpperBnds, 207
discreteStateVars, 207
histogramUncBinPairs, 206
histogramUncPointPairs, 206
idVariables, 204
lognormalUncDistLowerBnds, 205
lognormalUncDistUpperBnds, 205
lognormalUncErrFacts, 205
lognormalUncMeans, 205
lognormalUncStdDevs, 205
loguniformUncDistLowerBnds, 206
loguniformUncDistUpperBnds, 206
normalUncDistLowerBnds, 205
normalUncDistUpperBnds, 205
normalUncMeans, 205
normalUncStdDevs, 205
num_continuous_variables, 203
num_discrete_variables, 203
num_variables, 203
numContinuousDesVars, 204
numContinuousStateVars, 204
numDiscreteDesVars, 204
numDiscreteStateVars, 204
numHistogramUncVars, 204
numLognormalUncVars, 204
numLoguniformUncVars, 204
numNormalUncVars, 204
numUniformUncVars, 204
numWeibullUncVars, 204
operator=, 203
operator==, 203
read, 203
state, 203
uncertain, 203
uncertainCorrelations, 206
uncertainDistLowerBnds, 206
uncertainDistUpperBnds, 206
uncertainLabels, 206
uncertainVars, 206
uniformUncDistLowerBnds, 205
uniformUncDistUpperBnds, 205
weibullUncAlphas, 206
weibullUncBetas, 206
write, 203
DataVariables, 203
dbFnsList
DakotaModel, 135
dbLocked
ProblemDescDB, 319
dbResponseList
DakotaModel, 135
deallocate_arrays
SOLBase, 346
debugFlag
DakotaInterface, 110
debugOutput
DakotaIterator, 116
defaultASV
ApplicationInterface, 49
define_filenames
AnalysisCode, 39
DELFUN
CONMINOptimizer, 74
KrigApprox, 243
deltaList
DakotaModel, 135
deltasPerVariable
DataMethod, 195
ParamStudy, 313
derived_asynch_compute_response
DakotaModel, 133
HierLayeredModel, 240
NestedModel, 272
SingleModel, 333
SurrLayeredModel, 357
derived_compute_response
DakotaModel, 133
HierLayeredModel, 240
NestedModel, 272
SingleModel, 333
SurrLayeredModel, 357
derived_init_communicators
DakotaModel, 133
HierLayeredModel, 239
NestedModel, 272
SingleModel, 333
SurrLayeredModel, 358
derived_map
ApplicationInterface, 45
DirectFnApplicInterface, 208
ForkApplicInterface, 219
SysCallApplicInterface, 364
derived_map_ac
DirectFnApplicInterface, 209
derived_map_asynch
ApplicationInterface, 45
DirectFnApplicInterface, 208
ForkApplicInterface, 219
SysCallApplicInterface, 364
derived_map_if
DirectFnApplicInterface, 209
derived_map_of

DirectFnApplicInterface, 209
derived_master_overload
DakotaModel, 129
HierLayeredModel, 239
NestedModel, 269
SingleModel, 333
SurrLayeredModel, 358
derived_synch
ApplicationInterface, 45
DirectFnApplicInterface, 208
ForkApplicInterface, 219
SysCallApplicInterface, 364
derived_synch_kernel
ForkApplicInterface, 220
SysCallApplicInterface, 365
derived_synch_nowait
ApplicationInterface, 45
DirectFnApplicInterface, 208
ForkApplicInterface, 219
SysCallApplicInterface, 364
derived_synchronize
DakotaModel, 133
HierLayeredModel, 240
NestedModel, 272
SingleModel, 333
SurrLayeredModel, 357
derived_synchronize_nowait
DakotaModel, 133
HierLayeredModel, 240
NestedModel, 272
SingleModel, 333
SurrLayeredModel, 358
derived_synchronous_local_analysis
ApplicationInterface, 45
DirectFnApplicInterface, 208
ForkApplicInterface, 219
SysCallApplicInterface, 364
design
DataVariables, 203
designModel
NonDOptStrategy, 287
DF
CONMINOptimizer, 77
KrigApprox, 248
DirectFnApplicInterface
~DirectFnApplicInterface, 208
cantilever, 210
cyl_head, 210
derived_map, 208
derived_map_ac, 209
derived_map_asynch, 208
derived_map_if, 209
derived_map_of, 209
derived_synch, 208
derived_synch_nowait, 208
derived_synchronous_local_analysis, 208
DirectFnApplicInterface, 208
directFnASV, 210
directFnResponse, 210
directFnVars, 210
fnGrads, 210
fnHessians, 210
fnVals, 209
gradFlag, 209
hessFlag, 209
iFilterName, 209
mc_api_run, 211
numFns, 209
numGradVars, 209
numVars, 209
oFilterName, 209
overlay_response, 209
pxcFile, 209
rosenbrock, 210
salinas, 211
set_local_data, 209
text_book, 210
text_book1, 210
text_book2, 210
text_book3, 210
text_book_ouu, 210
xVect, 209
DirectFnApplicInterface, 208
directFnASV
DirectFnApplicInterface, 210
directFnResponse
DirectFnApplicInterface, 210
directFnVars
DirectFnApplicInterface, 210
discrete_lower_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 32
DakotaModel, 131
DakotaVarConstraints, 168
FundamentalVarConstraints, 223
MergedVarConstraints, 259
discrete_upper_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 32
DakotaModel, 131
DakotaVarConstraints, 169
FundamentalVarConstraints, 223
MergedVarConstraints, 259
discrete_variable_labels
AllMergedVariables, 29
AllVariables, 36
DakotaModel, 130
DakotaVariables, 175

FundamentalVariables, 228
MergedVariables, 263
discrete_variables
AllMergedVariables, 28
AllVariables, 35
DakotaModel, 130
DakotaVariables, 175
FundamentalVariables, 227
MergedVariables, 262
discreteAppFlag
SGOPTOptimizer, 328
discreteDesignLabels
DataVariables, 205
FundamentalVariables, 229
discreteDesignLowerBnds
DataVariables, 204
FundamentalVarConstraints, 225
discreteDesignUpperBnds
DataVariables, 205
FundamentalVarConstraints, 225
discreteDesignVars
DataVariables, 204
FundamentalVariables, 229
discreteFlag
DakotaVarConstraints, 170
discreteStateLabels
DataVariables, 207
FundamentalVariables, 230
discreteStateLowerBnds
DataVariables, 207
FundamentalVarConstraints, 225
discreteStateUpperBnds
DataVariables, 207
FundamentalVarConstraints, 225
discreteStateVars
DataVariables, 207
FundamentalVariables, 229
DoEval
COLINApplication, 62
SGOPTApplication, 326
dotFDSinfo
DOTOptimizer, 214
dotInfo
DOTOptimizer, 214
dotMethod
DOTOptimizer, 214
DOTOptimizer, 212
~DOTOptimizer, 212
allocate_workspace, 212
constraintMappingIndices, 215
constraintMappingMultipliers, 215
constraintMappingOffsets, 215
dotFDSinfo, 214
dotInfo, 214
dotMethod, 214
DOTOptimizer, 212
find_optimum, 212
intCntlParmArray, 214
intWorkSpace, 213
intWorkSpaceSize, 213
localConstraintValues, 215
optimizationType, 214
printControl, 214
realCntlParmArray, 214
realWorkSpace, 213
realWorkSpaceSize, 213
draw_surface
DakotaApproximation, 86
dummyFlag
ParallelLibrary, 302
duplication_detect
ApplicationInterface, 52
dv
AllMergedVariables, 28
AllVariables, 35
DakotaModel, 130
DakotaVariables, 174
FundamentalVariables, 227
MergedVariables, 262

emptyIntVector
DakotaVarConstraints, 171
DakotaVariables, 177
emptyRealVector
DakotaVarConstraints, 171
DakotaVariables, 177
emptyStringArray
DakotaVariables, 177
enroll
GetLongOpt, 234
enroll_done
GetLongOpt, 233
entries
DakotaList, 122
ePSAOptimizer
SGOPTOptimizer, 329
erfInverse
NonDAdvMeanValue, 279
error_ofstream
ParallelLibrary, 302
ErrorTable
msg, 216
rc, 216
ErrorTable, 216
eval_analysis_communicator_rank
ParallelLibrary, 301
eval_analysis_communicator_size
ParallelLibrary, 301

eval_analysis_inter_communicator
ParallelLibrary, 301
eval_analysis_inter_communicators
ParallelLibrary, 301
eval_analysis_intra_communicator
ParallelLibrary, 301
eval_analysis_message_pass
ParallelLibrary, 301
eval_analysis_split_flag
ParallelLibrary, 301
eval_id
ParamResponsePair, 310
evalAnalysisCommRank
ParallelLibrary, 305
evalAnalysisCommSize
ParallelLibrary, 305
evalAnalysisInterComm
ParallelLibrary, 305
evalAnalysisInterComms
ParallelLibrary, 305
evalAnalysisIntraComm
ApplicationInterface, 47
ParallelLibrary, 305
evalAnalysisMessagePass
ParallelLibrary, 305
evalAnalysisSplitFlag
ParallelLibrary, 305
evalCacheFlag
ApplicationInterface, 49
DataInterface, 186
evalComm
ApplicationInterface, 47
evalCommRank
ApplicationInterface, 46
ParallelLibrary, 304
evalCommSize
ApplicationInterface, 46
ParallelLibrary, 304
evalDedicatedMasterFlag
ParallelLibrary, 305
evalDedMasterFlag
ApplicationInterface, 46
evalId
ParamResponsePair, 311
evalIdList
ForkApplicInterface, 220
HierLayeredModel, 239
evalIntraComm
ParallelLibrary, 304
evalMasterFlag
ParallelLibrary, 304
evalMessagePass
ApplicationInterface, 46
evalScheduling
ApplicationInterface, 48
DataInterface, 186
evalServerId
ApplicationInterface, 46
ParallelLibrary, 305
evalServers
DataInterface, 186
evaluate_parameter_sets
DakotaIterator, 118
evaluation_communicator_rank
ParallelLibrary, 300
evaluation_communicator_size
ParallelLibrary, 300
evaluation_dedicated_master_flag
ParallelLibrary, 301
evaluation_intra_communicator
ParallelLibrary, 300
evaluation_master_flag
ParallelLibrary, 300
evaluation_server_id
ParallelLibrary, 300
evaluation_servers
ParallelLibrary, 300
expandAfterSuccess
DataMethod, 193
expansionFlag
DataMethod, 193
expansionOrder
DataMethod, 194
expansionTerms
DataMethod, 194
exploratoryMoves
DataMethod, 193
SGOPTOptimizer, 328

f_of_x_array
KrigingSurf, 250
failAction
ApplicationInterface, 49
DataInterface, 186
failCountList
SysCallApplicInterface, 365
failIdList
SysCallApplicInterface, 365
failRecoveryFnVals
ApplicationInterface, 49
failRetryLimit
ApplicationInterface, 49
fd_gradients
DakotaModel, 137
FDCH
CONMINOptimizer, 73
KrigApprox, 243
FDCHM

CONMINOptimizer, 73
KrigApprox, 243
fdnlf1
SNLLOptimizer, 342
fdnlf1Con
SNLLOptimizer, 342
fdStepSize
DataResponses, 197
fileNameKey
AnalysisCode, 41
fileSaveFlag
AnalysisCode, 40
DataInterface, 185
fileTagFlag
AnalysisCode, 40
DataInterface, 185
finalPoint
DataMethod, 194
ParamStudy, 313
finalStatistics
DakotaNonD, 141
find
DakotaList, 124
find_coefficients
ANNSurf, 42
DakotaApproximation, 86
HermiteSurf, 236
KrigingSurf, 250
MARSSurf, 257
RespSurf, 321
TaylorSurf, 366
find_optimum
COLINOptimizer, 65
CONMINOptimizer, 72
DakotaOptimizer, 143
DOTOptimizer, 212
NPSOLOptimizer, 294
rSQPOptimizer, 323
SGOPTOptimizer, 330
SNLLOptimizer, 341
find_optimum_on_model
NPSOLOptimizer, 294
find_optimum_on_user_functions
NPSOLOptimizer, 294
finiteDiffSS
DakotaModel, 135
finiteDiffStepSize
DakotaIterator, 116
finiteDiffType
DakotaIterator, 115
fitInactiveCLowerBnds
LayeredModel, 253
fitInactiveCUpperBnds
LayeredModel, 253
fitInactiveCVars
LayeredModel, 253
fitInactiveDLowerBnds
LayeredModel, 253
fitInactiveDUpperBnds
LayeredModel, 253
fitInactiveDVars
LayeredModel, 253
fixedSeedFlag
DataMethod, 194
flags
MARSSurf, 257
flush
CommandShell, 69
fn_tags
DakotaResponse, 150
fnEvalCntr
SOLBase, 348
fnEvalId
DakotaInterface, 109
fnGrads
DirectFnApplicInterface, 210
fnHessians
DirectFnApplicInterface, 210
fnTags
DakotaResponseRep, 155
fnVals
DirectFnApplicInterface, 209
force_rebuild
LayeredModel, 255
fork_application
ForkApplicInterface, 220
fork_program
ForkAnalysisCode, 217
ForkAnalysisCode
~ForkAnalysisCode, 217
argList, 217
argument_list, 217
fork_program, 217
ForkAnalysisCode, 217
tag_argument_list, 217
ForkAnalysisCode, 217
check_status, 218
ForkApplicInterface
~ForkApplicInterface, 219
derived_map, 219
derived_map_asynch, 219
derived_synch, 219
derived_synch_kernel, 220
derived_synch_nowait, 219
derived_synchronous_local_analysis, 219
evalIdList, 220
ForkApplicInterface, 219
forkSimulator, 220

processIdList, 220
ForkApplicInterface, 219
asynchronous_local_analyses, 221
fork_application, 220
serve_analyses_asynch, 221
synchronous_local_analyses, 221
forkSimulator
ForkApplicInterface, 220
free_analysis_communicators
ParallelLibrary, 297
free_communicators
ApplicationInterface, 44
DakotaInterface, 108
DakotaModel, 129
DakotaStrategy, 163
HierLayeredModel, 239
NestedModel, 270
SingleModel, 334
SurrLayeredModel, 356
free_evaluation_communicators
ParallelLibrary, 297
free_iterator_communicators
ParallelLibrary, 297
fRinvVector
KrigApprox, 246
function_gradients
DakotaResponse, 151
function_hessians
DakotaResponse, 151
function_values
DakotaResponse, 150, 151
FunctionCompare
FunctionCompare, 222
operator(), 222
search_val, 222
testFunction, 222
FunctionCompare, 222
functionGradients
DakotaResponseRep, 155
functionHessians
DakotaResponseRep, 155
functionPrecision
DataMethod, 191
functionSurfaceCoeffs
ApproximationInterface, 56
functionSurfaces
ApproximationInterface, 57
functionValues
DakotaResponseRep, 155
FundamentalVarConstraints
~FundamentalVarConstraints, 223
all_continuous_lower_bounds, 224
all_continuous_upper_bounds, 224
all_discrete_lower_bounds, 224
all_discrete_upper_bounds, 224
continuous_lower_bounds, 223
continuous_upper_bounds, 223
continuousDesignLowerBnds, 224
continuousDesignUpperBnds, 225
continuousStateLowerBnds, 225
continuousStateUpperBnds, 225
discrete_lower_bounds, 223
discrete_upper_bounds, 223
discreteDesignLowerBnds, 225
discreteDesignUpperBnds, 225
discreteStateLowerBnds, 225
discreteStateUpperBnds, 225
FundamentalVarConstraints, 225
inactive_continuous_lower_bounds, 223, 224
inactive_continuous_upper_bounds, 224
inactive_discrete_lower_bounds, 224
inactive_discrete_upper_bounds, 224
nonDFlag, 224
read, 224
uncertainDistLowerBnds, 225
uncertainDistUpperBnds, 225
write, 224
FundamentalVarConstraints, 223
FundamentalVarConstraints, 225
FundamentalVariables
~FundamentalVariables, 227
acv, 228
adv, 228
all_continuous_variable_labels, 228
all_continuous_variables, 228
all_discrete_variable_labels, 228
all_discrete_variables, 228
continuous_variable_labels, 227, 228
continuous_variables, 227
continuousDesignLabels, 229
continuousDesignVars, 229
continuousStateLabels, 230
continuousStateVars, 229
copy_rep, 229
cv, 227
discrete_variable_labels, 228
discrete_variables, 227
discreteDesignLabels, 229
discreteDesignVars, 229
discreteStateLabels, 230
discreteStateVars, 229
dv, 227
FundamentalVariables, 227, 230
inactive_continuous_variables, 228
inactive_discrete_variables, 228
nonDFlag, 229
read, 228, 229

read_annotated, 228
tv, 227
uncertainLabels, 230
uncertainVars, 229
write, 228, 229
write_annotated, 229
FundamentalVariables, 227
FundamentalVariables, 230
operator==, 230
fValueVector
KrigApprox, 246

G1
CONMINOptimizer, 77
KrigApprox, 248
G2
CONMINOptimizer, 77
KrigApprox, 248
gammaContract
SurrBasedOptStrategy, 351
gammaExpand
SurrBasedOptStrategy, 351
gammaNoChange
SurrBasedOptStrategy, 351
get
DakotaList, 123
get_approx
DakotaApproximation, 88
get_bool
ProblemDescDB, 317
get_chaos
HermiteSurf, 236
get_db_list_nodes
ProblemDescDB, 316
get_dia
ProblemDescDB, 317
get_dil
ProblemDescDB, 317
get_div
ProblemDescDB, 317
get_dra
ProblemDescDB, 317
get_drm
ProblemDescDB, 317
get_drv
ProblemDescDB, 317
get_drva
ProblemDescDB, 317
get_dsa
ProblemDescDB, 317
get_dsl
ProblemDescDB, 317
get_gradient
DakotaApproximation, 85
RespSurf, 321
TaylorSurf, 366
get_int
ProblemDescDB, 317
get_interface
DakotaInterface, 111
get_iterator
DakotaIterator, 119
get_min_point
COLINOptimizer, 64
get_model
DakotaModel, 137
get_num_chaos
HermiteSurf, 236
get_real
ProblemDescDB, 317
get_sizet
ProblemDescDB, 317
get_source_pair
ApplicationInterface, 48
get_strategy
DakotaStrategy, 163
get_string
ProblemDescDB, 317
get_value
ANNSurf, 42
DakotaApproximation, 85
HermiteSurf, 236
KrigingSurf, 250
MARSSurf, 257
RespSurf, 321
TaylorSurf, 366
get_var_constraints
DakotaVarConstraints, 173
get_variables
DakotaVariables, 179
GetLongOpt
~GetLongOpt, 232
basename, 233
enroll_done, 233
GetLongOpt, 233
last, 233
optmarker, 233
pname, 233
setcell, 233
table, 233
usage, 232
ustring, 233
GetLongOpt, 232
enroll, 234
GetLongOpt, 233
parse, 234
retrieve, 234
usage, 234

getRe
CtelRegexp, 79
getStatus
CtelRegexp, 79
getStatusMsg
CtelRegexp, 79
globalApproxFlag
SurrBasedOptStrategy, 352
gradFlag
DirectFnApplicInterface, 209
gradient_concurrency
DakotaModel, 132
gradient_method
DakotaModel, 132
gradientFlag
DakotaApproximation, 86
SurrBasedOptStrategy, 352
gradientTolerance
DataMethod, 191
gradientType
DakotaIterator, 115
DataResponses, 197
gradType
DakotaModel, 135
gradVector
DakotaApproximation, 86
graphics2D
DakotaGraphics, 104
graphicsCntr
DakotaGraphics, 104
graphicsFlag
ApproximationInterface, 56
DakotaStrategy, 161
DataStrategy, 199
gridHostNames
DataInterface, 185
gridProcsPerHost
DataInterface, 185

hard_convergence_check
SurrBasedOptStrategy, 353
headerFlag
ApplicationInterface, 49
HermiteSurf
~HermiteSurf, 236
approximation_coefficients, 236
chaosCoeffs, 237
chaosSamples, 237
find_coefficients, 236
get_chaos, 236
get_num_chaos, 236
get_value, 236
HermiteSurf, 236
highestOrder, 237
numChaos, 237
required_samples, 236
HermiteSurf, 236
hessFlag
DirectFnApplicInterface, 209
hessianType
DakotaIterator, 115
DataResponses, 197
hierarchApproxFlag
SurrBasedOptStrategy, 352
HierLayeredModel
~HierLayeredModel, 238
build_approximation, 238
derived_init_communicators, 239
derived_master_overload, 239
evalIdList, 239
free_communicators, 239
HierLayeredModel, 238
highFidelityModel, 239
highFidResponse, 239
local_eval_synchronization, 238
lowFidelityInterface, 239
new_eval_counter, 239
serve, 239
stop_servers, 239
subordinate_model, 238
synchronize_nowait_completions, 239
total_eval_counter, 239
HierLayeredModel, 238
derived_asynch_compute_response, 240
derived_compute_response, 240
derived_synchronize, 240
derived_synchronize_nowait, 240
highestOrder
HermiteSurf, 237
NonDPCESampling, 289
highFidelityInterfacePtr
DataInterface, 187
highFidelityModel
HierLayeredModel, 239
highFidResponse
HierLayeredModel, 239
histogramBinPairs
DakotaNonD, 140
histogramPointPairs
DakotaNonD, 140
histogramUncBinPairs
DataVariables, 206
histogramUncPointPairs
DataVariables, 206
historyDuplicateIds
ApplicationInterface, 49
historyDuplicateResponses
ApplicationInterface, 49

IC
CONMINOptimizer, 78
KrigApprox, 249
ICNDIR
KrigApprox, 245
idAnalytic
DakotaModel, 135
DataResponses, 197
idInterface
DataInterface, 184
idMethod
DataMethod, 189
idNumerical
DataResponses, 197
idResponses
DataResponses, 197
idrKeywordTable
keywordtable.C, 369
idVariables
DataVariables, 204
iFilterName
AnalysisCode, 40
DirectFnApplicInterface, 209
iFlag
KrigApprox, 249
IGOTO
KrigApprox, 245
impFactor
NonDAdvMeanValue, 280
inactive_continuous_lower_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 32, 33
DakotaModel, 131
DakotaVarConstraints, 169
FundamentalVarConstraints, 223, 224
MergedVarConstraints, 259, 260
inactive_continuous_upper_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 33
DakotaModel, 131
DakotaVarConstraints, 169
FundamentalVarConstraints, 224
MergedVarConstraints, 260
inactive_continuous_variables
AllMergedVariables, 29
AllVariables, 36
DakotaModel, 131
DakotaVariables, 175
FundamentalVariables, 228
MergedVariables, 263
inactive_discrete_lower_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 33
DakotaModel, 131
DakotaVarConstraints, 169
FundamentalVarConstraints, 224
MergedVarConstraints, 260
inactive_discrete_upper_bounds
AllMergedVarConstraints, 26
AllVarConstraints, 33
DakotaModel, 131
DakotaVarConstraints, 169
FundamentalVarConstraints, 224
MergedVarConstraints, 260
inactive_discrete_variables
AllMergedVariables, 29
AllVariables, 36
DakotaModel, 131
DakotaVariables, 175
FundamentalVariables, 228
MergedVariables, 263
inBuf
DakotaBiStream, 99
index
DakotaList, 124, 125
INFOG
KrigApprox, 245
informResult
SOLBase, 347
init_analysis_communicators
ParallelLibrary, 307
init_communicators
ApplicationInterface, 44
DakotaInterface, 108
DakotaModel, 137
DakotaStrategy, 163
init_evaluation_communicators
ParallelLibrary, 306
init_fn
SNLLBase, 336
init_iterator_communicators
ParallelLibrary, 306
init_serial
ApplicationInterface, 50
DakotaInterface, 108
initDelta
DataMethod, 192
initialize_graphics
DakotaStrategy, 163
initialMapList
DakotaModel, 135
initialPoint
NPSOLOptimizer, 295
ParamStudy, 313
input_filter_name
AnalysisCode, 39
inputFilter
DataInterface, 184

insert
    DakotaList, 124
insert_node
    ProblemDescDB, 317, 318
intCntlParmArray
    DOTOptimizer, 214
interface_id
    DakotaResponse, 150
    ParamResponsePair, 310
interface_kwhandler
    ProblemDescDB, 318
interface_synchronization
    ApplicationInterface, 44
    DakotaInterface, 108
interface_type
    DakotaInterface, 108
interfaceId
    DakotaResponseRep, 155
interfaceIter
    ProblemDescDB, 319
interfaceList
    ProblemDescDB, 319
interfacePointer
    DataMethod, 189
    NestedModel, 271
interfaceRep
    DakotaInterface, 110
interfaceResponse
    NestedModel, 271
interfaceSynchronization
    ApplicationInterface, 49
    DataInterface, 185
interfaceType
    DakotaInterface, 109
    DataInterface, 184
intervalType
    DakotaModel, 135
    DataResponses, 197
intProblem
    SGOPTOptimizer, 329
intWorkSpace
    DOTOptimizer, 213
    SOLBase, 347
intWorkSpaceSize
    DOTOptimizer, 213
    SOLBase, 347
invcorrelMatrix
    KrigApprox, 246
iPivotVector
    KrigApprox, 246
IPRINT
    CONMINOptimizer, 73
    KrigApprox, 243
irecv_ea
    ParallelLibrary, 298
irecv_ie
    ParallelLibrary, 298
irecv_si
    ParallelLibrary, 298
is_null
    DakotaIterator, 114
    DakotaModel, 132
ISC
    CONMINOptimizer, 78
    KrigApprox, 248
isEmpty
    DakotaList, 123
isend_ea
    ParallelLibrary, 298
isend_ie
    ParallelLibrary, 298
isend_si
    ParallelLibrary, 298
isNull
    DakotaString, 165
ITER
    KrigApprox, 245
iterated_mean_value
    NonDAdvMeanValue, 278
iterator_communicator
    DakotaStrategy, 159
iterator_communicator_rank
    ParallelLibrary, 299
iterator_communicator_size
    DakotaStrategy, 160
    ParallelLibrary, 299
iterator_dedicated_master_flag
    DakotaInterface, 109
    ParallelLibrary, 300
iterator_eval_communicator_rank
    ParallelLibrary, 300
iterator_eval_communicator_size
    ParallelLibrary, 300
iterator_eval_inter_communicator
    ParallelLibrary, 300
iterator_eval_inter_communicators
    ParallelLibrary, 300
iterator_eval_intra_communicator
    ParallelLibrary, 300
iterator_eval_message_pass
    ParallelLibrary, 300
iterator_eval_split_flag
    ParallelLibrary, 300
iterator_intra_communicator
    ParallelLibrary, 299
iterator_master_flag
    ParallelLibrary, 299
iterator_response_results

DACEIterator, 81
DakotaIterator, 113
DakotaNonD, 139
DakotaOptLeastSq, 146
ParamStudy, 312
iterator_server_id
ParallelLibrary, 300
iterator_servers
ParallelLibrary, 299
iterator_variable_results
DACEIterator, 81
DakotaIterator, 113
DakotaOptLeastSq, 146
ParamStudy, 312
iteratorComm
DakotaStrategy, 160
iteratorCommRank
ApplicationInterface, 46
DakotaStrategy, 160
ParallelLibrary, 303
iteratorCommSize
ApplicationInterface, 46
DakotaStrategy, 160
ParallelLibrary, 304
iteratorDedicatedMasterFlag
ParallelLibrary, 304
iteratorDedMasterFlag
DakotaInterface, 109
iteratorEvalCommRank
ParallelLibrary, 304
iteratorEvalCommSize
ParallelLibrary, 305
iteratorEvalInterComm
ParallelLibrary, 304
iteratorEvalInterComms
ParallelLibrary, 304
iteratorEvalIntraComm
ParallelLibrary, 304
iteratorEvalMessagePass
ParallelLibrary, 304
iteratorEvalSplitFlag
ParallelLibrary, 304
iteratorIntraComm
ParallelLibrary, 303
iteratorMasterFlag
ParallelLibrary, 303
iteratorRep
DakotaIterator, 117
iteratorScheduling
DataStrategy, 200
iteratorServerId
ConcurrentStrategy, 71
ParallelLibrary, 304
iteratorServers
DataStrategy, 199
iterMax
SurrBasedOptStrategy, 351
ITMAX
CONMINOptimizer, 73
KrigApprox, 243
ITRM
KrigApprox, 244
ivec
ColinPoint, 66
iworkVector
KrigApprox, 246

jacUToX
NonDAdvMeanValue, 284
jacXToU
NonDAdvMeanValue, 283
jacXToZ
NonDAdvMeanValue, 283
jacZToX
NonDAdvMeanValue, 283

keywordtable.C, 369
idrKeywordTable, 369
KrigApprox
~KrigApprox, 242
ABOBJ1, 244
ALPHAX, 244
betaHat, 245
conminInfo, 243
conminSingleArray, 242
conminThetaLowerBnds, 244
conminThetaUpperBnds, 244
conminThetaVars, 244
constraintVector, 246
correlationMatrix, 246
CTL, 243
CTLMIN, 243
CTMIN, 243
DABFUN, 243
DELFUN, 243
FDCH, 243
FDCHM, 243
fRinvVector, 246
fValueVector, 246
ICNDIR, 245
IGOTO, 245
INFOG, 245
invcorrelMatrix, 246
iPivotVector, 246
IPRINT, 243
ITER, 245
ITMAX, 243
ITRM, 244

iworkVector, 246
KrigApprox, 242
LINOBJ, 244
maxLikelihoodEst, 245
ModelBuild, 242
NAC, 245
NACMX1, 244
NFDG, 242
NSCAL, 244
NSIDE, 244
numcon, 242
numNewPts, 245
numSampQuad, 245
PHI, 244
rhsTermsVector, 246
rXhatVector, 246
THETA, 244
thetaLoBndVector, 245
thetaUpBndVector, 246
thetaVector, 245
workVector, 246
workVectorQuad, 246
xMatrix, 245
xNewVector, 245
yfbRinvVector, 246
yfbVector, 246
yNewVector, 245
yValueVector, 245

KrigApprox, 242
A, 248
B, 248
C, 248
CT, 247
DF, 248
G1, 248
G2, 248
IC, 249
iFlag, 249
ISC, 248
ModelApply, 247
MS1, 248
N1, 247
N2, 247
N3, 247
N4, 247
N5, 247
S, 247
SCAL, 248

krigingCorrelations
DataInterface, 187

KrigingSurf
~KrigingSurf, 250
correlationVector, 250
f_of_x_array, 250
find_coefficients, 250
get_value, 250
KrigingSurf, 250
krigObject, 250
required_samples, 250
runConminFlag, 251
x_matrix, 250

KrigingSurf, 250

krigObject
KrigingSurf, 250

last
GetLongOpt, 233

LayeredModel
~LayeredModel, 252
apply_correction, 252
approxType, 253
auto_correction, 252
badScalingFlag, 254
betaApproxCenterGrads, 254
betaApproxCenterVals, 254
betaCenterPt, 254
betaFns, 254
betaGrads, 254
check_submodel_compatibility, 252
correctedResponseArray, 252
correctedResponseList, 253
correctionComputed, 254
correctionOrder, 253
correctionType, 253
fitInactiveCLowerBnds, 253
fitInactiveCUpperBnds, 253
fitInactiveCVars, 253
fitInactiveDLowerBnds, 253
fitInactiveDUpperBnds, 253
fitInactiveDVars, 253
LayeredModel, 252
offsetValues, 254
rawCVarsList, 253
scaleFactors, 254

LayeredModel, 252
approxBuilds, 255
autoCorrection, 255
compute_correction, 254
force_rebuild, 255
refitInactive, 255

least_sq_eval
NLSSOLLeastSq, 275

length
DakotaArray, 91
DakotaBaseVector, 96

lenPRPairMessage
ApplicationInterface, 47

lenResponseMessage

ApplicationInterface, 47
lenVarsASVMessage
ApplicationInterface, 47
lenVarsMessage
ApplicationInterface, 47
lin_approx_constraint_eval
NonDAdvMeanValue, 282
lin_approx_objective_eval
NonDAdvMeanValue, 281
lin_eq_jac
rSQPOptimizer, 323
lin_eq_targ
rSQPOptimizer, 323
lin_ineq_jac
rSQPOptimizer, 323
lin_ineq_lb
rSQPOptimizer, 323
lin_ineq_ub
rSQPOptimizer, 323
linConGenerator
SGOPTOptimizer, 328
linConstraintArraySize
SOLBase, 347
linConstraintMatrixF77
SOLBase, 347
linear_eq_constraint_coeffs
DakotaModel, 132
DakotaVarConstraints, 170
linear_eq_constraint_targets
DakotaModel, 132
DakotaVarConstraints, 170
linear_ineq_constraint_coeffs
DakotaModel, 131
DakotaVarConstraints, 170
linear_ineq_constraint_lower_bounds
DakotaModel, 132
DakotaVarConstraints, 170
linear_ineq_constraint_upper_bounds
DakotaModel, 132
DakotaVarConstraints, 170
linearEqConstraintCoeffs
DakotaOptLeastSq, 148
DakotaVarConstraints, 171
DataMethod, 191
linearEqConstraintTargets
DakotaVarConstraints, 171
linearEqTargets
DakotaOptLeastSq, 148
DataMethod, 191
linearIneqConstraintCoeffs
DakotaOptLeastSq, 147
DakotaVarConstraints, 170
DataMethod, 191
linearIneqConstraintLowerBnds
DakotaVarConstraints, 171
linearIneqConstraintUpperBnds
DakotaVarConstraints, 171
linearIneqLowerBnds
DakotaOptLeastSq, 147
DataMethod, 191
linearIneqUpperBnds
DakotaOptLeastSq, 148
DataMethod, 191
lineSearchTolerance
DataMethod, 191
LINOBJ
KrigApprox, 244
listOfPoints
DataMethod, 195
ParamStudy, 313
local_eval_synchronization
DakotaModel, 137
HierLayeredModel, 238
SingleModel, 333
localApproxFlag
SurrBasedOptStrategy, 352
localConstraintValues
CONMINOptimizer, 75
DOTOptimizer, 215
localSearchProb
MultilevelOptStrategy, 267
lognormalDistLowerBnds
DakotaNonD, 140
lognormalDistUpperBnds
DakotaNonD, 140
lognormalErrFacts
DakotaNonD, 140
lognormalMeans
DakotaNonD, 140
lognormalStdDevs
DakotaNonD, 140
lognormalUncDistLowerBnds
DataVariables, 205
lognormalUncDistUpperBnds
DataVariables, 205
lognormalUncErrFacts
DataVariables, 205
lognormalUncMeans
DataVariables, 205
lognormalUncStdDevs
DataVariables, 205
loguniformDistLowerBnds
DakotaNonD, 140
loguniformDistUpperBnds
DakotaNonD, 140
loguniformUncDistLowerBnds
DataVariables, 206
loguniformUncDistUpperBnds

DataVariables, 206
lower
DakotaString, 166
lowerBounds
NPSOLOptimizer, 295
lowFidelityInterface
HierLayeredModel, 239
lowFidelityInterfacePtr
DataInterface, 187

main
main.C, 370
restart_util.C, 372
main.C, 370
main, 370
write_precision, 370
manage_asv
DakotaModel, 138
manage_failure
ApplicationInterface, 44
manage_inputs
ProblemDescDB, 320
manage_linear_constraints
DakotaVarConstraints, 173
manage_outputs_restart
ParallelLibrary, 307
map
ApplicationInterface, 50
ApproximationInterface, 55
DakotaInterface, 107
map_response
COLINApplication, 63
marsObject
MARSSurf, 257
MARSSurf, 257
~MARSSurf, 257
find_coefficients, 257
flags, 257
get_value, 257
marsObject, 257
MARSSurf, 257
required_samples, 257
match
CtelRegexp, 79
maxConcurrency
DakotaIterator, 115
maxCPUTime
DataMethod, 192
maxFunctionEvals
DakotaIterator, 115
maxFunctionEvaluations
DataMethod, 190
maximum_concurrency
DakotaIterator, 114
DakotaModel, 128
SurrLayeredModel, 358
maxIterations
DakotaIterator, 115
DataMethod, 190
maxLikelihoodEst
KrigApprox, 245
maxStep
DataMethod, 191
mc_api_run
DirectFnApplicInterface, 211
mean95CIDeltas
DakotaNonD, 141
mean_value
NonDAdvMeanValue, 278
meanStats
DakotaNonD, 141
medianFnVals
NonDAdvMeanValue, 280
merged_integer_list
DakotaModel, 132
DakotaVariables, 176
mergedDesignLabels
MergedVariables, 264
mergedDesignLowerBnds
MergedVarConstraints, 260
mergedDesignUpperBnds
MergedVarConstraints, 260
mergedDesignVars
MergedVariables, 264
mergedIntegerList
DakotaVariables, 176
mergedStateLabels
MergedVariables, 264
mergedStateLowerBnds
MergedVarConstraints, 261
mergedStateUpperBnds
MergedVarConstraints, 261
mergedStateVars
MergedVariables, 264
MergedVarConstraints
~MergedVarConstraints, 259
all_continuous_lower_bounds, 260
all_continuous_upper_bounds, 260
all_discrete_lower_bounds, 260
all_discrete_upper_bounds, 260
continuous_lower_bounds, 259
continuous_upper_bounds, 259
discrete_lower_bounds, 259
discrete_upper_bounds, 259
inactive_continuous_lower_bounds, 259, 260
inactive_continuous_upper_bounds, 260
inactive_discrete_lower_bounds, 260

inactive_discrete_upper_bounds, 260
mergedDesignLowerBnds, 260
mergedDesignUpperBnds, 260
mergedStateLowerBnds, 261
mergedStateUpperBnds, 261
MergedVarConstraints, 261
read, 260
uncertainDistLowerBnds, 261
uncertainDistUpperBnds, 261
write, 260
MergedVarConstraints, 259
MergedVarConstraints, 261
MergedVariables
~MergedVariables, 262
acv, 263
adv, 263
all_continuous_variable_labels, 263
all_continuous_variables, 263
all_discrete_variable_labels, 263
all_discrete_variables, 263
continuous_variable_labels, 262, 263
continuous_variables, 262
copy_rep, 264
cv, 262
discrete_variable_labels, 263
discrete_variables, 262
dv, 262
inactive_continuous_variables, 263
inactive_discrete_variables, 263
mergedDesignLabels, 264
mergedDesignVars, 264
mergedStateLabels, 264
mergedStateVars, 264
MergedVariables, 262, 265
operator==, 264
read, 263, 264
read_annotated, 263
tv, 262
uncertainLabels, 264
uncertainVars, 264
write, 263, 264
write_annotated, 263
MergedVariables, 262
MergedVariables, 265
meritFn
DataMethod, 191
message_lengths
DakotaModel, 132
messageLengths
DakotaModel, 134
method_kwhandler
ProblemDescDB, 318
method_name
DakotaIterator, 114
methodIter
ProblemDescDB, 319
methodList
MultilevelOptStrategy, 267
ProblemDescDB, 319
methodName
DakotaIterator, 115
DataMethod, 189
methodOutput
DataMethod, 190
methodPointer
DataStrategy, 200
methodSource
DakotaIterator, 116
DataResponses, 197
methodSrc
DakotaModel, 135
mfcn
SNLLBase, 336
minimize_residuals
DakotaLeastSq, 120
NLSSOLLeastSq, 275
SNLLLeastSq, 338
minimum_samples
ApproximationInterface, 55
DakotaInterface, 108
minMaxType
DataMethod, 191
minSamples
ApproximationInterface, 56
minTrustRegionFactor
SurrBasedOptStrategy, 351
mixedGradAnalyticIds
DakotaIterator, 116
mixedGradNumericalIds
DakotaIterator, 116
model_
rSQPOptimizer, 323
model_type
DakotaModel, 132
ModelApply
KrigApprox, 247
modelAutoGraphicsFlag
DakotaModel, 134
ModelBuild
KrigApprox, 242
modelCenterFile
DataInterface, 185
modelRep
DakotaModel, 134
modelType
DakotaModel, 134
DataMethod, 190
modified_parameters_filename

AnalysisCode, 39
modified_results_filename
AnalysisCode, 39
modifiedParamsFileName
AnalysisCode, 40
modifiedResFileName
AnalysisCode, 40
mostProbPointU
NonDAdvMeanValue, 281
mostProbPointX
NonDAdvMeanValue, 281
mpirun_flag
ParallelLibrary, 299
mpirunFlag
DakotaStrategy, 161
ParallelLibrary, 302
MS1
CONMINOptimizer, 77
KrigApprox, 248
msg
ErrorTable, 216
multi_objective_modify
DakotaOptimizer, 145
multi_objective_weights
DakotaIterator, 114
DakotaOptimizer, 143
multi_proc_eval_flag
DakotaInterface, 109
multidim_loop
ParamStudy, 313
multilevelGlobalMethodPointer
DataStrategy, 200
multilevelLocalMethodPointer
DataStrategy, 200
multilevelLSProb
DataStrategy, 200
multilevelMethodList
DataStrategy, 200
MultilevelOptStrategy
~MultilevelOptStrategy, 266
localSearchProb, 267
methodList, 267
MultilevelOptStrategy, 266
multiLevelType, 267
numIterators, 267
progressMetric, 267
progressThreshold, 267
run_strategy, 266
selectedIterators, 267
strategy_response_results, 266
strategy_variable_results, 266
userDefinedModels, 267
MultilevelOptStrategy, 266
run_coupled, 267
run_uncoupled, 268
run_uncoupled_adaptive, 268
multilevelProgThresh
DataStrategy, 200
multiLevelType
MultilevelOptStrategy, 267
multilevelType
DataStrategy, 200
multiObjectiveWeights
DataResponses, 197
multiobjModifyPtr
COLINApplication, 62
SGOPTApplication, 326
multiObjWeights
DACEIterator, 83
DakotaOptimizer, 144
ParamStudy, 314
multiObjWts
SurrBasedOptStrategy, 352
multiProcAnalysisFlag
ApplicationInterface, 47
multiProcEvalFlag
DakotaInterface, 109
multiStartFlag
ConcurrentStrategy, 70
mutationDimRate
DataMethod, 192
mutationMinScale
DataMethod, 192
mutationPopRate
DataMethod, 192
mutationRange
DataMethod, 193
mutationScale
DataMethod, 192
mutationType
DataMethod, 193

N1
CONMINOptimizer, 76
KrigApprox, 247
N2
CONMINOptimizer, 76
KrigApprox, 247
N3
CONMINOptimizer, 76
KrigApprox, 247
N4
CONMINOptimizer, 76
KrigApprox, 247
N5
CONMINOptimizer, 76
KrigApprox, 247
NAC

KrigApprox, 245
NACMX1
KrigApprox, 244
nestedFlag
ParamStudy, 313
NestedModel
~NestedModel, 269
asv_mapping, 270
completionList, 271
constrCoeffs, 271
derived_master_overload, 269
free_communicators, 270
interfacePointer, 271
interfaceResponse, 271
NestedModel, 269
new_eval_counter, 270
numInterfEqConstr, 271
numInterfIneqConstr, 271
numInterfObjFns, 271
numSubIteratorEqConstr, 270
numSubIteratorIneqConstr, 270
objCoeffs, 271
optionalInterface, 271
responseArray, 271
responseList, 271
serve, 270
stop_servers, 270
subIterator, 270
subordinate_model, 269
total_eval_counter, 270
NestedModel, 269
derived_asynch_compute_response, 272
derived_compute_response, 272
derived_init_communicators, 272
derived_synchronize, 272
derived_synchronize_nowait, 272
response_mapping, 273
subModel, 273
synchronize_nowait_completions, 272
new_eval_counter
DakotaInterface, 108
DakotaModel, 129
HierLayeredModel, 239
NestedModel, 270
SingleModel, 334
SurrLayeredModel, 356
newCenterFlag
SurrBasedOptStrategy, 352
newFnEvalId
DakotaInterface, 109
newSolnsGenerated
DataMethod, 192
next_eval
COLINApplication, 62
SGOPTApplication, 326
NFDG
CONMINOptimizer, 73
KrigApprox, 242
nlf0
SNLLOptimizer, 342
nlf0_evaluator
SNLLOptimizer, 344
nlf1
SNLLOptimizer, 342
nlf1_evaluator
SNLLOptimizer, 344
nlf1Con
SNLLOptimizer, 342
nlf2
SNLLLeastSq, 339
SNLLOptimizer, 342
nlf2_evaluator
SNLLOptimizer, 344
nlf2_evaluator_gn
SNLLLeastSq, 340
nlf2Con
SNLLLeastSq, 339
SNLLOptimizer, 342
nlfConstraint
SNLLLeastSq, 339
SNLLOptimizer, 342
nlfObjective
SNLLLeastSq, 338
SNLLOptimizer, 342
nlnConstraintArraySize
SOLBase, 347
nlp_
rSQPOptimizer, 323
nlpConstraint
SNLLLeastSq, 339
SNLLOptimizer, 342
NLSSOLLeastSq
~NLSSOLLeastSq, 275
least_sq_eval, 275
minimize_residuals, 275
NLSSOLLeastSq, 275
NLSSOLLeastSq, 275
NoDBBaseConstructor
NoDBBaseConstructor, 277
NoDBBaseConstructor, 277
nonAdaptiveFlag
DataMethod, 193
NonDAdvMeanValue
~NonDAdvMeanValue, 278
amvFlag, 281
cholCorrMatrix, 280
erfInverse, 279
impFactor, 280

iterated_mean_value, 278
mean_value, 278
medianFnVals, 280
mostProbPointU, 281
mostProbPointX, 281
NonDAdvMeanValue, 278
numLevels, 280
numRelEqConstr, 280
petraCorrMatrix, 280
petraProbLevels, 281
petraRespLevels, 281
print_iterator_results, 278
probLevels, 280
quantify_uncertainty, 278
ranVarMeans, 281
ranVarSigmas, 281
ranVarType, 281
reliabilityMethod, 280
respLevelCount, 281
staticFnGrads, 280
staticFnVals, 280
staticGlobalGradsU, 280
staticGlobalGradsX, 280
staticNumFuncs, 281
staticNumUncVars, 281
transUToX, 278

NonDAdvMeanValue, 278
- correctedRespLevel, 284
- jacUToX, 284
- jacXToU, 283
- jacXToZ, 283
- jacZToX, 283
- lin_approx_constraint_eval, 282
- lin_approx_objective_eval, 281
- transNataf, 284
- transUToX, 282
- transUToZ, 283
- transXToU, 282
- transXToZ, 282
- transZToU, 283

nonDFlag
- FundamentalVarConstraints, 224
- FundamentalVariables, 229

NonDLHSSampling
- ∼NonDLHSSampling, 285
- allVarsFlag, 285
- NonDLHSSampling, 286
- print_iterator_results, 285

NonDLHSSampling, 285
- NonDLHSSampling, 286
- quantify_uncertainty, 286

NonDOptStrategy
- ∼NonDOptStrategy, 287
- designModel, 287
- NonDOptStrategy, 287
- optIterator, 287
- run_strategy, 287
- strategy_response_results, 287
- strategy_variable_results, 287

NonDOptStrategy, 287

NonDPCESampling
- ∼NonDPCESampling, 289
- coeffArray, 289
- highestOrder, 289
- NonDPCESampling, 289
- numChaos, 289
- print_iterator_results, 289
- quantify_uncertainty, 289

NonDPCESampling, 289

NonDSampling
- ∼NonDSampling, 291
- allDataFlag, 292
- check_error, 292
- compute_statistics, 291
- NonDSampling, 293
- numActiveVars, 292
- numDesignVars, 292
- numLHSRuns, 292
- numObservations, 292
- numStateVars, 292
- originalSeed, 292
- print_statistics, 291
- randomSeed, 292
- run_lhs, 291
- sampleType, 292
- sampling_scheme, 291
- statsFlag, 292
- strategyFlag, 292
- varyPattern, 292

NonDSampling, 291
- NonDSampling, 293
- sampling_reset, 293

nonlin_eq_targ
- rSQPOptimizer, 323

nonlin_ineq_lb
- rSQPOptimizer, 323

nonlin_ineq_ub
- rSQPOptimizer, 323

nonlinearEqTargets
- DACEIterator, 83
- DakotaOptLeastSq, 147
- DataResponses, 197
- ParamStudy, 314

nonlinearIneqLowerBnds
- DACEIterator, 83
- DakotaOptLeastSq, 147
- DataResponses, 197
- ParamStudy, 314

nonlinearIneqUpperBnds
DACEIterator, 83
DakotaOptLeastSq, 147
DataResponses, 197
ParamStudy, 314
nonlinEqTargets
SurrBasedOptStrategy, 353
nonlinIneqLowerBnds
SurrBasedOptStrategy, 352
nonlinIneqUpperBnds
SurrBasedOptStrategy, 353
normalDistLowerBnds
DakotaNonD, 140
normalDistUpperBnds
DakotaNonD, 140
normalMeans
DakotaNonD, 139
normalStdDevs
DakotaNonD, 139
normalUncDistLowerBnds
DataVariables, 205
normalUncDistUpperBnds
DataVariables, 205
normalUncMeans
DataVariables, 205
normalUncStdDevs
DataVariables, 205
NPSOLOptimizer, 294
~NPSOLOptimizer, 294
find_optimum, 294
find_optimum_on_model, 294
find_optimum_on_user_functions, 294
initialPoint, 295
lowerBounds, 295
NPSOLOptimizer, 294
objective_eval, 295
setUpType, 295
upperBounds, 295
userConstraintEval, 295
userObjectiveEval, 295
NSCAL
KrigApprox, 244
NSIDE
KrigApprox, 244
num_active_variables
DakotaVarConstraints, 170
num_columns
DakotaMatrix, 126
num_continuous_variables
DataVariables, 203
num_discrete_variables
DataVariables, 203
num_functions
DakotaModel, 130
DakotaResponse, 150
num_integer_params
COLINApplication, 62
num_linear_eq_constraints
DakotaModel, 131
DakotaVarConstraints, 170
num_linear_ineq_constraints
DakotaModel, 131
DakotaVarConstraints, 169
num_objectives
rSQPOptimizer, 323
num_real_params
COLINApplication, 62
num_rows
DakotaMatrix, 126
num_variables
DakotaApproximation, 86
DataVariables, 203
numActiveVars
NonDSampling, 292
numAnalysisDrivers
ApplicationInterface, 47
numAnalysisServers
ApplicationInterface, 47
ParallelLibrary, 305
numberIterations
SOLBase, 347
numberRetained
DataMethod, 192
numCDV
AllVarConstraints, 34
AllVariables, 37
numChaos
HermiteSurf, 237
NonDPCESampling, 289
numCoeffs
RespSurf, 321
numcon
KrigApprox, 242
numConstraints
DakotaOptLeastSq, 147
numContinuousDesVars
DataVariables, 204
numContinuousStateVars
DataVariables, 204
numContinuousVars
DakotaIterator, 115
numCSV
AllVarConstraints, 34
AllVariables, 37
numCurrentPoints
DakotaApproximation, 86
numDACERuns
DACEIterator, 82

numDDV
AllVarConstraints, 34
AllVariables, 37
numDesignVars
NonDSampling, 292
numDiscreteDesVars
DataVariables, 204
numDiscreteStateVars
DataVariables, 204
numDiscreteVars
DakotaIterator, 115
numDSV
AllVarConstraints, 34
AllVariables, 37
numEvalServers
ApplicationInterface, 48
ParallelLibrary, 304
numFns
DakotaModel, 133
DirectFnApplicInterface, 209
SurrBasedOptStrategy, 352
numFunctions
DakotaIterator, 115
numGradVars
DakotaModel, 133
DirectFnApplicInterface, 209
numHistogramUncVars
DataVariables, 204
numHistogramVars
DakotaNonD, 141
numInterfEqConstr
NestedModel, 271
numInterfIneqConstr
NestedModel, 271
numInterfObjFns
NestedModel, 271
numIteratorJobs
ConcurrentStrategy, 70
numIterators
MultilevelOptStrategy, 267
numIteratorServers
BranchBndStrategy, 59
ConcurrentStrategy, 70
ParallelLibrary, 303
numLeastSqTerms
DakotaLeastSq, 120
DataResponses, 196
numLevels
NonDAdvMeanValue, 280
numLHSRuns
NonDSampling, 292
numLinearConstraints
DakotaOptLeastSq, 148
numLinearEqConstraints
DakotaOptLeastSq, 148
DakotaVarConstraints, 170
numLinearIneqConstraints
DakotaOptLeastSq, 147
DakotaVarConstraints, 170
numLognormalUncVars
DataVariables, 204
numLognormalVars
DakotaNonD, 141
numLoguniformUncVars
DataVariables, 204
numLoguniformVars
DakotaNonD, 141
numMapsList
DakotaModel, 135
numNewPts
KrigApprox, 245
numNodeSamples
BranchBndStrategy, 59
numNonlinCons
COLINApplication, 62
SGOPTApplication, 326
numNonlinearConstraints
DakotaOptLeastSq, 147
numNonlinearEqConstraints
DACEIterator, 83
DakotaOptLeastSq, 147
DataResponses, 196
ParamStudy, 314
numNonlinearIneqConstraints
DACEIterator, 83
DakotaOptLeastSq, 147
DataResponses, 196
ParamStudy, 314
numNonlinEqConstr
SurrBasedOptStrategy, 352
numNonlinIneqConstr
SurrBasedOptStrategy, 352
numNormalUncVars
DataVariables, 204
numNormalVars
DakotaNonD, 140
numObjectiveFunctions
DACEIterator, 82
DakotaOptimizer, 144
DataResponses, 196
ParamStudy, 314
numObjFns
COLINApplication, 61
SGOPTApplication, 326
SurrBasedOptStrategy, 352
numObservations
NonDSampling, 292
numPartitions

DataMethod, 193
numPrograms
AnalysisCode, 40
numRelEqConstr
NonDAdvMeanValue, 280
numResponseFunctions
DakotaNonD, 141
DataResponses, 197
numRootSamples
BranchBndStrategy, 59
numSamples
DACEIterator, 82
DakotaApproximation, 86
DataMethod, 194
numSampQuad
KrigApprox, 245
numStateVars
NonDSampling, 292
numSteps
DataMethod, 195
ParamStudy, 313
numSubIteratorEqConstr
NestedModel, 270
numSubIteratorIneqConstr
NestedModel, 270
numSymbols
DACEIterator, 82
DataMethod, 194
numUncertainVars
DakotaNonD, 141
numUniformUncVars
DataVariables, 204
numUniformVars
DakotaNonD, 141
numUV
AllVarConstraints, 34
AllVariables, 37
numVars
DakotaApproximation, 86
DakotaIterator, 115
DirectFnApplicInterface, 209
SurrBasedOptStrategy, 352
numWeibullUncVars
DataVariables, 204
numWeibullVars
DakotaNonD, 141

objCoeffs
NestedModel, 271
objective_eval
NPSOLOptimizer, 295
occurrencesOf
DakotaList, 125
offsetValues
LayeredModel, 254
oFilterName
AnalysisCode, 40
DirectFnApplicInterface, 209
operator const char *
DakotaString, 166
operator T *
DakotaArray, 92
DakotaVector, 180
operator!=
DakotaResponse, 152
DakotaVariables, 177
ParamResponsePair, 310
operator()
DakotaArray, 92
DakotaBaseVector, 96
FunctionCompare, 222
SortCompare, 349
operator<<
CommandShell, 68
DakotaBoStream, 101–103
operator=
CtelRegexp, 80
DakotaApproximation, 88
DakotaArray, 90, 92
DakotaBaseVector, 94
DakotaInterface, 111
DakotaIterator, 118
DakotaList, 122
DakotaMatrix, 127
DakotaModel, 137
DakotaResponse, 150
DakotaStrategy, 162
DakotaString, 165
DakotaVarConstraints, 172
DakotaVariables, 179
DakotaVector, 180, 182
DataInterface, 184
DataMethod, 189
DataResponses, 196
DataStrategy, 199
DataVariables, 203
ParamResponsePair, 309
SurrogateDataPoint, 360
operator==
AllMergedVariables, 30
AllVariables, 38
DakotaResponse, 152
DakotaResponseRep, 156
DakotaVariables, 177
DataInterface, 184
DataMethod, 189
DataResponses, 196
DataVariables, 203

FundamentalVariables, 230
MergedVariables, 264
ParamResponsePair, 310
SurrogateDataPoint, 360
operator>>
DakotaBiStream, 98–100
operator[]
DakotaArray, 90, 92
DakotaBaseVector, 94–96
DakotaList, 125
optbcfdnewton
SNLLOptimizer, 343
optbcnewton
SNLLLeastSq, 339
SNLLOptimizer, 343
optbcqnewton
SNLLOptimizer, 343
optcg
SNLLOptimizer, 342
optfdnewton
SNLLOptimizer, 343
optfdnips
SNLLOptimizer, 343
optimizationType
CONMINOptimizer, 75
DOTOptimizer, 214
optimizer
COLINOptimizer, 64
optionalInterface
NestedModel, 271
optionalInterfaceResponsesPointer
DataMethod, 190
optIterator
NonDOptStrategy, 287
optmarker
GetLongOpt, 233
optnewton
SNLLLeastSq, 339
SNLLOptimizer, 343
optnips
SNLLLeastSq, 339
SNLLOptimizer, 343
optpds
SNLLOptimizer, 342
optqnewton
SNLLOptimizer, 343
optqnips
SNLLOptimizer, 343
originalSeed
DACEIterator, 82
NonDSampling, 292
outBuf
DakotaBoStream, 102
output_filter_name
AnalysisCode, 39
output_ofstream
ParallelLibrary, 302
outputFilter
DataInterface, 184
overlay
DakotaResponse, 152
DakotaResponseRep, 155
overlay_response
DirectFnApplicInterface, 209
ownMPIFlag
ParallelLibrary, 302

parallel_library
ProblemDescDB, 316
parallel_time
ParallelLibrary, 299
parallelism_levels
ParallelLibrary, 299
parallelismLevels
ParallelLibrary, 302
parallelLib
AnalysisCode, 41
ApplicationInterface, 45
DakotaModel, 134
DakotaStrategy, 160
ProblemDescDB, 319
ParallelLibrary
~ParallelLibrary, 297
analysis_communicator_rank, 301
analysis_communicator_size, 301
analysis_intra_communicator, 301
analysis_master_flag, 301
analysis_server_id, 301
analysis_servers, 301
analysisCommRank, 305
analysisCommSize, 305
analysisIntraComm, 305
analysisMasterFlag, 305
analysisServerId, 305
bcast, 298
dummyFlag, 302
error_ofstream, 302
eval_analysis_communicator_rank, 301
eval_analysis_communicator_size, 301
eval_analysis_inter_communicator, 301
eval_analysis_inter_communicators, 301
eval_analysis_intra_communicator, 301
eval_analysis_message_pass, 301
eval_analysis_split_flag, 301
evalAnalysisCommRank, 305
evalAnalysisCommSize, 305
evalAnalysisInterComm, 305
evalAnalysisInterComms, 305

evalAnalysisIntraComm, 305
evalAnalysisMessagePass, 305
evalAnalysisSplitFlag, 305
evalCommRank, 304
evalCommSize, 304
evalDedicatedMasterFlag, 305
evalIntraComm, 304
evalMasterFlag, 304
evalServerId, 305
evaluation_communicator_rank, 300
evaluation_communicator_size, 300
evaluation_dedicated_master_flag, 301
evaluation_intra_communicator, 300
evaluation_master_flag, 300
evaluation_server_id, 300
evaluation_servers, 300
free_analysis_communicators, 297
free_evaluation_communicators, 297
free_iterator_communicators, 297
irecv_ea, 298
irecv_ie, 298
irecv_si, 298
isend_ea, 298
isend_ie, 298
isend_si, 298
iterator_communicator_rank, 299
iterator_communicator_size, 299
iterator_dedicated_master_flag, 300
iterator_eval_communicator_rank, 300
iterator_eval_communicator_size, 300
iterator_eval_inter_communicator, 300
iterator_eval_inter_communicators, 300
iterator_eval_intra_communicator, 300
iterator_eval_message_pass, 300
iterator_eval_split_flag, 300
iterator_intra_communicator, 299
iterator_master_flag, 299
iterator_server_id, 300
iterator_servers, 299
iteratorCommRank, 303
iteratorCommSize, 304
iteratorDedicatedMasterFlag, 304
iteratorEvalCommRank, 304
iteratorEvalCommSize, 305
iteratorEvalInterComm, 304
iteratorEvalInterComms, 304
iteratorEvalIntraComm, 304
iteratorEvalMessagePass, 304
iteratorEvalSplitFlag, 304
iteratorIntraComm, 303
iteratorMasterFlag, 303
iteratorServerId, 304
mpirun_flag, 299
mpirunFlag, 302
numAnalysisServers, 305
numEvalServers, 304
numIteratorServers, 303
output_ofstream, 302
ownMPIFlag, 302
parallel_time, 299
parallelism_levels, 299
parallelismLevels, 302
ParallelLibrary, 306
print_configuration, 297
procsPerAnalysis, 305
procsPerEval, 304
procsPerIterator, 303
recv_ea, 298
recv_ie, 298
recv_si, 298
send_ea, 298
send_ie, 298
send_si, 298
split_communicator_dedicated_master, 302
split_communicator_peer_partition, 302
startClock, 303
startCPUTime, 303
startMPITime, 303
startWCTime, 303
stdErrorFlag, 303
stdOutputFlag, 302
strategy_dedicated_master_flag, 299
strategy_iterator_communicator_rank, 300
strategy_iterator_communicator_size, 300
strategy_iterator_inter_communicator, 299
strategy_iterator_inter_communicators, 299
strategy_iterator_intra_communicator, 299
strategy_iterator_message_pass, 299
strategy_iterator_split_flag, 299
strategyDedicatedMasterFlag, 303
stratIteratorCommRank, 304
stratIteratorCommSize, 304
stratIteratorInterComm, 303
stratIteratorInterComms, 303
stratIteratorIntraComm, 303
stratIteratorMessagePass, 303
stratIteratorSplitFlag, 303
waitall, 299
world_rank, 299
world_size, 299
worldRank, 302
worldSize, 302

ParallelLibrary, 297
close_streams, 308
init_analysis_communicators, 307
init_evaluation_communicators, 306
init_iterator_communicators, 306
manage_outputs_restart, 307

ParallelLibrary, 306
resolve_inputs, 308
parameterSets
ConcurrentStrategy, 70
parametersFile
DataInterface, 185
parametersFileName
AnalysisCode, 40
parametersFNameList
AnalysisCode, 41
ParamResponsePair
~ParamResponsePair, 309
active_set_vector, 310
eval_id, 310
interface_id, 310
operator
=, 310
operator=, 309
operator==, 310
ParamResponsePair, 309, 311
prp_parameters, 310
prp_response, 310
prPairParameters, 310
prPairResponse, 310
read, 309
read_annotated, 309
write, 309, 310
write_annotated, 309
write_tabular, 309
ParamResponsePair, 309
evalId, 311
ParamResponsePair, 311
ParamStudy
~ParamStudy, 312
bestObjectiveFn, 314
bestResponses, 314
bestVariables, 314
bestViolations, 314
centered_loop, 313
compute_vector_steps, 312
deltasPerVariable, 313
finalPoint, 313
initialPoint, 313
iterator_response_results, 312
iterator_variable_results, 312
listOfPoints, 313
multidim_loop, 313
multiObjWeights, 314
nestedFlag, 313
nonlinearEqTargets, 314
nonlinearIneqLowerBnds, 314
nonlinearIneqUpperBnds, 314
numNonlinearEqConstraints, 314
numNonlinearIneqConstraints, 314
numObjectiveFunctions, 314
numSteps, 313
ParamStudy, 312
percentDelta, 313
print_iterator_results, 312
psCounter, 314
pStudyType, 313
recurse, 313
sample, 312
stepLength, 313
stepVector, 313
update_best, 313
variablePartitions, 314
vector_loop, 312
ParamStudy, 312
run_iterator, 315
paramStudyType
DataMethod, 194
parse
GetLongOpt, 234
patternBasis
DataMethod, 193
patternSearchOptimizer
SGOPTOptimizer, 329
penaltyParameter
SurrBasedOptStrategy, 351
percentDelta
DataMethod, 195
ParamStudy, 313
petraCorrMatrix
NonDAdvMeanValue, 280
petraProbLevels
NonDAdvMeanValue, 281
petraRespLevels
NonDAdvMeanValue, 281
pGAIntOptimizer
SGOPTOptimizer, 329
pGARealOptimizer
SGOPTOptimizer, 329
PHI
KrigApprox, 244
picoComm
BranchBndStrategy, 59
picoCommRank
BranchBndStrategy, 59
picoCommSize
BranchBndStrategy, 60
picoListOfIntegers
BranchBndStrategy, 60
picoLowerBnds
BranchBndStrategy, 60
picoUpperBnds
BranchBndStrategy, 60
pname

GetLongOpt, 233
polyCoeffs
RespSurf, 321
polynomialOrder
DataInterface, 187
polyOrder
RespSurf, 322
populate_gradient_vars
DakotaIterator, 119
populationSize
DataMethod, 192
post_instantiate
SNLLBase, 335
post_run
SNLLBase, 335
pre_instantiate
SNLLBase, 335
pre_run
SNLLBase, 335
primaryCoeffs
DataMethod, 190
print
DakotaArray, 91
DakotaList, 122
DakotaMatrix, 126
DakotaVector, 181, 182
print_annotated
DakotaVector, 181
print_aprepro
DakotaVector, 181
print_configuration
ParallelLibrary, 297
print_iterator_results
DACEIterator, 81
DakotaIterator, 113
DakotaLeastSq, 121
DakotaOptimizer, 144
NonDAdvMeanValue, 278
NonDLHSSampling, 285
NonDPCESampling, 289
ParamStudy, 312
print_partial
DakotaVector, 181
print_partial_aprepro
DakotaVector, 181
print_restart
restart_util.C, 371
print_restart_tabular
restart_util.C, 372
print_statistics
NonDSampling, 291
printControl
CONMINOptimizer, 75
DOTOptimizer, 214
prob_desc_db
DakotaModel, 132
DakotaStrategy, 164
probabilityLevels
DataMethod, 194
probDescDB
DakotaIterator, 115
DakotaModel, 134
DakotaStrategy, 160
problem
COLINOptimizer, 64
ProblemDescDB
~ProblemDescDB, 316
build_label, 318
build_labels, 318
build_labels_partial, 319
check_input, 316
dbLocked, 319
get_bool, 317
get_db_list_nodes, 316
get_dia, 317
get_dil, 317
get_div, 317
get_dra, 317
get_drm, 317
get_drv, 317
get_drva, 317
get_dsa, 317
get_dsl, 317
get_int, 317
get_real, 317
get_sizet, 317
get_string, 317
insert_node, 317, 318
interface_kwhandler, 318
interfaceIter, 319
interfaceList, 319
method_kwhandler, 318
methodIter, 319
methodList, 319
parallel_library, 316
parallelLib, 319
ProblemDescDB, 316
receive_db_buffer, 318
responses_kwhandler, 318
responsesIter, 319
responsesList, 319
send_db_buffer, 318
set_db_interface_node, 316
set_db_list_nodes, 316
set_db_responses_node, 316
set_other_list_nodes, 318
strategy_kwhandler, 318
strategyCntr, 319

strategySpec, 319
variables_kwhandler, 318
variablesIter, 319
variablesList, 319
ProblemDescDB, 316
manage_inputs, 320
set_db_model_type, 320
probLevels
NonDAdvMeanValue, 280
probMoreThanThresh
DakotaNonD, 141
processIdList
ForkApplicInterface, 220
procsPerAnalysis
ApplicationInterface, 48
DataInterface, 185
ParallelLibrary, 305
procsPerEval
ParallelLibrary, 304
procsPerIterator
ParallelLibrary, 303
program_names
AnalysisCode, 39
programNames
AnalysisCode, 40
progressMetric
MultilevelOptStrategy, 267
progressThreshold
MultilevelOptStrategy, 267
prp_parameters
ParamResponsePair, 310
prp_response
ParamResponsePair, 310
prPairParameters
ParamResponsePair, 310
prPairResponse
ParamResponsePair, 310
psCounter
ParamStudy, 314
pStudyType
ParamStudy, 313
purge_inactive
DakotaResponse, 152
DakotaResponseRep, 155
pxcFile
DirectFnApplicInterface, 209

quantify_uncertainty
DakotaNonD, 139
NonDAdvMeanValue, 278
NonDLHSSampling, 286
NonDPCESampling, 289
quietFlag
DakotaInterface, 110
DakotaModel, 135
quietOutput
DakotaIterator, 116

r
CtelRegexp, 80
randomizeOrderFlag
DataMethod, 193
randomSeed
DACEIterator, 82
DataMethod, 194
NonDSampling, 292
ranVarMeans
NonDAdvMeanValue, 281
ranVarSigmas
NonDAdvMeanValue, 281
ranVarType
NonDAdvMeanValue, 281
rawCVarsList
LayeredModel, 253
rawResponseArray
DakotaInterface, 112
rawResponseList
DakotaInterface, 112
rc
ErrorTable, 216
read
AllMergedVarConstraints, 27
AllMergedVariables, 29, 30
AllVarConstraints, 33
AllVariables, 36, 37
DakotaArray, 91
DakotaList, 122
DakotaMatrix, 126
DakotaResponse, 151
DakotaResponseRep, 156–158
DakotaVarConstraints, 169
DakotaVariables, 175, 176
DakotaVector, 180, 181
DataInterface, 184
DataMethod, 189
DataResponses, 196
DataStrategy, 199
DataVariables, 203
FundamentalVarConstraints, 224
FundamentalVariables, 228, 229
MergedVarConstraints, 260
MergedVariables, 263, 264
ParamResponsePair, 309
read_annotated
AllMergedVariables, 29
AllVariables, 36
DakotaResponse, 151
DakotaResponseRep, 157

DakotaVariables, 176
DakotaVector, 181
FundamentalVariables, 228
MergedVariables, 263
ParamResponsePair, 309
read_data
DakotaResponse, 152
DakotaResponseRep, 155
read_neutral
restart_util.C, 372
read_partial
DakotaVector, 181
read_restart_evals
CommandLineHandler, 67
read_results_file
AnalysisCode, 39
read_tabular
DakotaResponse, 151
DakotaResponseRep, 157
DakotaVector, 181
realCntlParmArray
DOTOptimizer, 214
realProblem
SGOPTOptimizer, 329
realWorkSpace
DOTOptimizer, 213
SOLBase, 347
realWorkSpaceSize
DOTOptimizer, 213
SOLBase, 347
receive_db_buffer
ProblemDescDB, 318
recoveryFnVals
DataInterface, 186
recurse
ParamStudy, 313
recv_ea
ParallelLibrary, 298
recv_ie
ParallelLibrary, 298
recv_si
ParallelLibrary, 298
referenceCount
DakotaApproximation, 87
DakotaInterface, 110
DakotaIterator, 117
DakotaModel, 134
DakotaResponseRep, 155
DakotaStrategy, 161
DakotaVarConstraints, 171
DakotaVariables, 177
refitInactive
LayeredModel, 255
reliabilityMethod
DataMethod, 194
NonDAdvMeanValue, 280
remove
DakotaList, 124
removeAt
DakotaList, 124
repair_restart
restart_util.C, 372
replacementType
DataMethod, 193
required_samples
ANNSurf, 42
DakotaApproximation, 85
HermiteSurf, 236
KrigingSurf, 250
MARSSurf, 257
RespSurf, 321
TaylorSurf, 366
reset
DakotaResponse, 152
DakotaResponseRep, 155
reshape
DakotaArray, 91
DakotaBaseVector, 96
reshape_2d
DakotaMatrix, 126
resolve_inputs
ParallelLibrary, 308
resolve_samples_symbols
DACEIterator, 84
respLevelCount
NonDAdvMeanValue, 281
response_mapping
NestedModel, 273
responseArray
DakotaModel, 135
NestedModel, 271
responseASV
DakotaResponseRep, 155
responseFn
SurrogateDataPoint, 360
responseGrad
SurrogateDataPoint, 360
responseLabels
DataResponses, 198
responseLevels
DataMethod, 194
responseList
DakotaModel, 135
NestedModel, 271
responseRep
DakotaResponse, 152
responses_kwhandler
ProblemDescDB, 318

responsesIter
ProblemDescDB, 319
responsesList
ProblemDescDB, 319
responsesPointer
DataMethod, 190
responseThresholds
DataMethod, 194
RespSurf
~RespSurf, 321
approximation_coefficients, 321
find_coefficients, 321
get_gradient, 321
get_value, 321
numCoeffs, 321
polyCoeffs, 321
polyOrder, 322
required_samples, 321
RespSurf, 321
RespSurf, 321
respThresh
DakotaNonD, 141
restart_util.C, 371
concatenate_restart, 372
main, 372
print_restart, 371
print_restart_tabular, 372
read_neutral, 372
repair_restart, 372
write_precision, 371
restartFileFlag
ApplicationInterface, 49
DataInterface, 186
results_fname
AnalysisCode, 39
resultsFile
DataInterface, 185
resultsFileName
AnalysisCode, 40
resultsFNameList
AnalysisCode, 41
retrieve
GetLongOpt, 234
retryLimit
DataInterface, 186
rhsTermsVector
KrigApprox, 246
rng
COLINOptimizer, 65
rosenbrock
DirectFnApplicInterface, 210
rSQPOptimizer
~rSQPOptimizer, 323
find_optimum, 323
lin_eq_jac, 323
lin_eq_targ, 323
lin_ineq_jac, 323
lin_ineq_lb, 323
lin_ineq_ub, 323
model_, 323
nlp_, 323
nonlin_eq_targ, 323
nonlin_ineq_lb, 323
nonlin_ineq_ub, 323
num_objectives, 323
rSQPOptimizer, 323
rSQPOptimizer, 323
run_coupled
MultilevelOptStrategy, 267
run_iterator
DACEIterator, 83
DakotaIterator, 118
DakotaLeastSq, 121
DakotaNonD, 139
DakotaOptimizer, 144
DakotaStrategy, 162
ParamStudy, 315
run_iterator_repartition
DakotaStrategy, 163
run_lhs
NonDSampling, 291
run_strategy
BranchBndStrategy, 59
ConcurrentStrategy, 70
DakotaStrategy, 159
MultilevelOptStrategy, 266
NonDOptStrategy, 287
SingleMethodStrategy, 331
SurrBasedOptStrategy, 353
run_uncoupled
MultilevelOptStrategy, 268
run_uncoupled_adaptive
MultilevelOptStrategy, 268
runConminFlag
KrigingSurf, 251
runningList
ApplicationInterface, 50
rvec
ColinPoint, 66
rXhatVector
KrigApprox, 246

S
CONMINOptimizer, 77
KrigApprox, 247
s
SNLLBase, 336
salinas

DirectFnApplicInterface, 211
sample
ParamStudy, 312
sampleReuse
ApproximationInterface, 56
sampleReuseFile
ApproximationInterface, 56
sampleType
DataMethod, 194
NonDSampling, 292
sampling_reset
DACEIterator, 81
DakotaIterator, 114
NonDSampling, 293
sampling_scheme
DACEIterator, 81
DakotaIterator, 114
NonDSampling, 291
SCAL
CONMINOptimizer, 77
KrigApprox, 248
scaleFactors
LayeredModel, 254
search_val
FunctionCompare, 222
searchMethod
DataMethod, 191
SNLLBase, 336
searchSchemeSize
DataMethod, 192
secondaryCoeffs
DataMethod, 190
selectedIterator
BranchBndStrategy, 59
ConcurrentStrategy, 70
SingleMethodStrategy, 331
SurrBasedOptStrategy, 351
selectedIterators
MultilevelOptStrategy, 267
selectionPressure
DataMethod, 193
self_schedule_analyses
ApplicationInterface, 51
self_schedule_evaluations
ApplicationInterface, 52
send_db_buffer
ProblemDescDB, 318
send_ea
ParallelLibrary, 298
send_ie
ParallelLibrary, 298
send_si
ParallelLibrary, 298
serve
DakotaModel, 129
HierLayeredModel, 239
NestedModel, 270
SingleModel, 334
SurrLayeredModel, 356
serve_analyses_asynch
ForkApplicInterface, 221
serve_analyses_synch
ApplicationInterface, 51
serve_evaluations
ApplicationInterface, 51
DakotaInterface, 107
serve_evaluations_asynch
ApplicationInterface, 53
serve_evaluations_peer
ApplicationInterface, 54
serve_evaluations_synch
ApplicationInterface, 53
set_bounds
DakotaApproximation, 86
set_db_interface_node
ProblemDescDB, 316
set_db_list_nodes
ProblemDescDB, 316
set_db_model_type
ProblemDescDB, 320
set_db_responses_node
ProblemDescDB, 316
set_initial_point
COLINOptimizer, 64
set_local_data
DirectFnApplicInterface, 209
set_method_options
COLINOptimizer, 64
SGOPTOptimizer, 330
set_options
SOLBase, 346
set_other_list_nodes
ProblemDescDB, 318
set_rng
COLINOptimizer, 64
set_standard_method_options
COLINOptimizer, 65
setcell
GetLongOpt, 233
setUpType
NPSOLOptimizer, 295
SGOPTApplication, 325
~SGOPTApplication, 325
activeSetVector, 325
copy, 325
dakota_asynch_flag, 326
dakotaCompletionList, 326
dakotaModelAsynchFlag, 325

dakotaResponseList, 325
DoEval, 326
multiobjModifyPtr, 326
next_eval, 326
numNonlinCons, 326
numObjFns, 326
SGOPTApplication, 325
synchronize, 326
userDefinedModel, 325
sgoptApplication
SGOPTOptimizer, 330
SGOPTOptimizer, 328
~SGOPTOptimizer, 330
aPPSOptimizer, 329
baseOptimizer, 329
discreteAppFlag, 328
ePSAOptimizer, 329
exploratoryMoves, 328
find_optimum, 330
intProblem, 329
linConGenerator, 328
patternSearchOptimizer, 329
pGAIntOptimizer, 329
pGARealOptimizer, 329
realProblem, 329
set_method_options, 330
sgoptApplication, 330
SGOPTOptimizer, 330
sMCrealOptimizer, 329
sWOptimizer, 329
show_data_3d
DakotaGraphics, 105
silentFlag
DakotaInterface, 109
DakotaModel, 135
silentOutput
DakotaIterator, 116
SingleMethodStrategy
~SingleMethodStrategy, 331
run_strategy, 331
selectedIterator, 331
SingleMethodStrategy, 331
strategy_response_results, 331
strategy_variable_results, 331
userDefinedModel, 331
SingleMethodStrategy, 331
SingleModel
~SingleModel, 333
derived_asynch_compute_response, 333
derived_compute_response, 333
derived_init_communicators, 333
derived_master_overload, 333
derived_synchronize, 333
derived_synchronize_nowait, 333
free_communicators, 334
local_eval_synchronization, 333
new_eval_counter, 334
serve, 334
SingleModel, 333
stop_servers, 334
synchronize_nowait_completions, 333
total_eval_counter, 334
userDefinedInterface, 334
SingleModel, 333
sMCrealOptimizer
SGOPTOptimizer, 329
SNLLBase, 335
~SNLLBase, 335
constantASVFlag, 336
copy_con_grad, 336
copy_con_hess, 336
copy_con_vals, 336
init_fn, 336
mfcn, 336
post_instantiate, 335
post_run, 335
pre_instantiate, 335
pre_run, 335
s, 336
searchMethod, 336
SNLLBase, 335
staticConEvalMode, 337
staticConEvalVars, 337
staticDebugOutput, 336
staticLastFnEvalLocn, 336
staticModeOverrideFlag, 336
staticNumNonlinearEqConstraints, 337
staticNumNonlinearIneqConstraints, 337
SNLLLeastSq
~SNLLLeastSq, 338
constraint2_evaluator_gn, 338
minimize_residuals, 338
nlf2, 339
nlf2Con, 339
nlfConstraint, 339
nlfObjective, 338
nlpConstraint, 339
optbcnewton, 339
optnewton, 339
optnips, 339
SNLLLeastSq, 338
theOptimizer, 339
SNLLLeastSq, 338
nlf2_evaluator_gn, 340
SNLLOptimizer, 341
~SNLLOptimizer, 341
constraint0_evaluator, 344
constraint1_evaluator, 344

constraint2_evaluator, 344
fdnlf1, 342
fdnlf1Con, 342
find_optimum, 341
nlf0, 342
nlf0_evaluator, 344
nlf1, 342
nlf1_evaluator, 344
nlf1Con, 342
nlf2, 342
nlf2_evaluator, 344
nlf2Con, 342
nlfConstraint, 342
nlfObjective, 342
nlpConstraint, 342
optbcfdnewton, 343
optbcnewton, 343
optbcqnewton, 343
optcg, 342
optfdnewton, 343
optfdnips, 343
optnewton, 343
optnips, 343
optpds, 342
optqnewton, 343
optqnips, 343
SNLLOptimizer, 341
theOptimizer, 342

soft_convergence_check
SurrBasedOptStrategy, 354

softConvCount
SurrBasedOptStrategy, 352

softConvLimit
SurrBasedOptStrategy, 352

SOLBase, 346
~SOLBase, 346
allocate_arrays, 346
allocate_workspace, 346
augment_bounds, 346
boundsArraySize, 347
cLambda, 347
constraint_eval, 347
constraintJacMatrixF77, 348
constraintState, 347
deallocate_arrays, 346
fnEvalCntr, 348
informResult, 347
intWorkSpace, 347
intWorkSpaceSize, 347
linConstraintArraySize, 347
linConstraintMatrixF77, 347
nlnConstraintArraySize, 347
numberIterations, 347
realWorkSpace, 347
realWorkSpaceSize, 347
set_options, 346
SOLBase, 346
staticConstrOffset, 348
staticMaxFnEvals, 348
staticSOLModel, 348
staticVendorNumericalGradFlag, 348
upperFactorHessianF77, 348

solnAccuracy
DataMethod, 192

sort
DakotaList, 124

SortCompare
operator(), 349
SortCompare, 349
sortFunction, 349

SortCompare, 349

sortFunction
SortCompare, 349

spawn_analysis
SysCallAnalysisCode, 363

spawn_application
SysCallApplicInterface, 365

spawn_evaluation
SysCallAnalysisCode, 363

spawn_input_filter
SysCallAnalysisCode, 363

spawn_output_filter
SysCallAnalysisCode, 363

speculativeFlag
DakotaOptLeastSq, 148
DataMethod, 190

split
CtelRegexp, 79

split_communicator_dedicated_master
ParallelLibrary, 302

split_communicator_peer_partition
ParallelLibrary, 302

startClock
ParallelLibrary, 303

startCPUTime
ParallelLibrary, 303

startMPITime
ParallelLibrary, 303

startWCTime
ParallelLibrary, 303

state
DataVariables, 203

static_schedule_evaluations
ApplicationInterface, 52

staticConEvalMode
SNLLBase, 337

staticConEvalVars
SNLLBase, 337

staticConstrOffset
SOLBase, 348
staticDebugOutput
SNLLBase, 336
staticFnGrads
NonDAdvMeanValue, 280
staticFnVals
NonDAdvMeanValue, 280
staticGlobalGradsU
NonDAdvMeanValue, 280
staticGlobalGradsX
NonDAdvMeanValue, 280
staticLastFnEvalLocn
SNLLBase, 336
staticMaxFnEvals
SOLBase, 348
staticModel
DakotaIterator, 116
staticModeOverrideFlag
SNLLBase, 336
staticMultiObjWeights
DakotaOptimizer, 144
staticNumContinuousVars
DakotaOptLeastSq, 148
staticNumFuncs
NonDAdvMeanValue, 281
staticNumLSqTerms
DakotaLeastSq, 121
staticNumNonlinearConstraints
DakotaOptLeastSq, 148
staticNumNonlinearEqConstraints
SNLLBase, 337
staticNumNonlinearIneqConstraints
SNLLBase, 337
staticNumObjFns
DakotaOptimizer, 144
staticNumUncVars
NonDAdvMeanValue, 281
staticSOLModel
SOLBase, 348
staticVendorNumericalGradFlag
SOLBase, 348
statsFlag
NonDSampling, 292
status
CtelRegexp, 80
statusMsg
CtelRegexp, 80
stdDevStats
DakotaNonD, 141
stdErrorFlag
ParallelLibrary, 303
stdOutputFlag
ParallelLibrary, 302
stepLength
DataMethod, 195
ParamStudy, 313
stepLenToBoundary
DataMethod, 191
stepVector
DataMethod, 194
ParamStudy, 313
stop_evaluation_servers
ApplicationInterface, 51
DakotaInterface, 107
stop_servers
DakotaModel, 129
HierLayeredModel, 239
NestedModel, 270
SingleModel, 334
SurrLayeredModel, 356
strategy_dedicated_master_flag
ParallelLibrary, 299
strategy_iterator_communicator_rank
ParallelLibrary, 300
strategy_iterator_communicator_size
ParallelLibrary, 300
strategy_iterator_inter_communicator
ParallelLibrary, 299
strategy_iterator_inter_communicators
ParallelLibrary, 299
strategy_iterator_intra_communicator
ParallelLibrary, 299
strategy_iterator_message_pass
ParallelLibrary, 299
strategy_iterator_split_flag
ParallelLibrary, 299
strategy_kwhandler
ProblemDescDB, 318
strategy_response_results
DakotaStrategy, 159
MultilevelOptStrategy, 266
NonDOptStrategy, 287
SingleMethodStrategy, 331
SurrBasedOptStrategy, 350
strategy_variable_results
DakotaStrategy, 159
MultilevelOptStrategy, 266
NonDOptStrategy, 287
SingleMethodStrategy, 331
SurrBasedOptStrategy, 350
strategyCntr
ProblemDescDB, 319
strategyDedicatedMasterFlag
ConcurrentStrategy, 71
ParallelLibrary, 303
strategyFlag
NonDSampling, 292

strategyName
DakotaStrategy, 160
strategyRep
DakotaStrategy, 161
strategySpec
ProblemDescDB, 319
strategyType
DataStrategy, 199
stratIteratorCommRank
ParallelLibrary, 304
stratIteratorCommSize
ParallelLibrary, 304
stratIteratorInterComm
ParallelLibrary, 303
stratIteratorInterComms
ParallelLibrary, 303
stratIteratorIntraComm
ParallelLibrary, 303
stratIteratorMessagePass
ParallelLibrary, 303
stratIteratorSplitFlag
ParallelLibrary, 303
strPattern
CtelRegexp, 80
subIterator
NestedModel, 270
subMethodPointer
DataMethod, 190
subModel
NestedModel, 273
subordinate_iterator
DakotaModel, 128
SurrLayeredModel, 355
subordinate_model
DakotaModel, 128
HierLayeredModel, 238
NestedModel, 269
SurrLayeredModel, 355
suppress_output_flag
AnalysisCode, 39
CommandShell, 68
suppressOutput
ApplicationInterface, 46
suppressOutputFlag
AnalysisCode, 40
CommandShell, 68
surrBasedOptConvTol
DataStrategy, 200
surrBasedOptMaxIterations
DataStrategy, 200
surrBasedOptSoftConvLimit
DataStrategy, 200
SurrBasedOptStrategy
~SurrBasedOptStrategy, 350
approximateModel, 351
bestResponses, 353
bestVariables, 353
constraintTol, 351
convergenceFlag, 351
convergenceTol, 351
correctionFlag, 352
daceCenterPtFlag, 352
gammaContract, 351
gammaExpand, 351
gammaNoChange, 351
globalApproxFlag, 352
gradientFlag, 352
hierarchApproxFlag, 352
iterMax, 351
localApproxFlag, 352
minTrustRegionFactor, 351
multiObjWts, 352
newCenterFlag, 352
nonlinEqTargets, 353
nonlinIneqLowerBnds, 352
nonlinIneqUpperBnds, 353
numFns, 352
numNonlinEqConstr, 352
numNonlinIneqConstr, 352
numObjFns, 352
numVars, 352
penaltyParameter, 351
selectedIterator, 351
softConvCount, 352
softConvLimit, 352
strategy_response_results, 350
strategy_variable_results, 350
SurrBasedOptStrategy, 350
trRatioContractValue, 351
trRatioExpandValue, 351
trustRegionFactor, 351
trustRegionSize, 351
SurrBasedOptStrategy, 350
compute_penalty_function, 353
hard_convergence_check, 353
run_strategy, 353
soft_convergence_check, 354
surrBasedOptTRContract
DataStrategy, 201
surrBasedOptTRContractTrigger
DataStrategy, 201
surrBasedOptTRExpand
DataStrategy, 201
surrBasedOptTRExpandTrigger
DataStrategy, 201
surrBasedOptTRInitSize
DataStrategy, 201
surrBasedOptTRMinSize

DataStrategy, 201
SurrLayeredModel
~SurrLayeredModel, 355
approximation_coefficients, 356
approxInterface, 356
daceIterator, 357
daceMethodPointer, 357
free_communicators, 356
new_eval_counter, 356
serve, 356
stop_servers, 356
subordinate_iterator, 355
subordinate_model, 355
SurrLayeredModel, 355
synchronize_nowait_completions, 356
total_eval_counter, 356
update_approximation, 356
SurrLayeredModel, 355
actualInterfacePointer, 359
actualModel, 359
build_approximation, 358
derived_asynch_compute_response, 357
derived_compute_response, 357
derived_init_communicators, 358
derived_master_overload, 358
derived_synchronize, 357
derived_synchronize_nowait, 358
maximum_concurrency, 358
SurrogateDataPoint
~SurrogateDataPoint, 360
continuousVars, 360
operator=, 360
operator==, 360
responseFn, 360
responseGrad, 360
SurrogateDataPoint, 360
SurrogateDataPoint, 360
sWOptimizer
SGOPTOptimizer, 329
synch
ApplicationInterface, 50
ApproximationInterface, 56
DakotaInterface, 107
synch_nowait
ApplicationInterface, 51
ApproximationInterface, 56
DakotaInterface, 107
synch_nowait_completions
DakotaInterface, 108
synchronize
COLINApplication, 62
DakotaModel, 130
SGOPTApplication, 326
synchronize_fd_gradients
DakotaModel, 138
synchronize_nowait
DakotaModel, 130
synchronize_nowait_completions
DakotaModel, 129
HierLayeredModel, 239
NestedModel, 272
SingleModel, 333
SurrLayeredModel, 356
synchronous_local_analyses
ForkApplicInterface, 221
synchronous_local_evaluations
ApplicationInterface, 53
SysCallAnalysisCode
~SysCallAnalysisCode, 362
command_usage, 362
commandUsage, 362
SysCallAnalysisCode, 362
SysCallAnalysisCode, 362
spawn_analysis, 363
spawn_evaluation, 363
spawn_input_filter, 363
spawn_output_filter, 363
SysCallApplicInterface
~SysCallApplicInterface, 364
derived_map, 364
derived_map_asynch, 364
derived_synch, 364
derived_synch_kernel, 365
derived_synch_nowait, 364
derived_synchronous_local_analysis, 364
failCountList, 365
failIdList, 365
spawn_application, 365
SysCallApplicInterface, 364
sysCallList, 365
sysCallSimulator, 365
system_call_file_test, 365
SysCallApplicInterface, 364
sysCallList
SysCallApplicInterface, 365
sysCallSimulator
SysCallApplicInterface, 365
system_call_file_test
SysCallApplicInterface, 365

table
GetLongOpt, 233
tabularDataFile
DakotaStrategy, 161
DataStrategy, 199
tabularDataFlag
DakotaGraphics, 104
DakotaStrategy, 161

DataStrategy, 199
tabularDataFStream
DakotaGraphics, 105
tag_argument_list
ForkAnalysisCode, 217
TaylorSurf
~TaylorSurf, 366
find_coefficients, 366
get_gradient, 366
get_value, 366
required_samples, 366
TaylorSurf, 366
TaylorSurf, 366
testClass
DakotaArray, 93
DakotaBoStream, 103
DakotaList, 123
DakotaMatrix, 127
DakotaString, 166
DakotaVector, 182
testFunction
FunctionCompare, 222
text_book
DirectFnApplicInterface, 210
text_book1
DirectFnApplicInterface, 210
text_book2
DirectFnApplicInterface, 210
text_book3
DirectFnApplicInterface, 210
text_book_ouu
DirectFnApplicInterface, 210
theOptimizer
SNLLLeastSq, 339
SNLLOptimizer, 342
THETA
KrigApprox, 244
thetaLoBndVector
KrigApprox, 245
thetaUpBndVector
KrigApprox, 246
thetaVector
KrigApprox, 245
threshDelta
DataMethod, 192
toLower
DakotaString, 165
total_eval_counter
DakotaInterface, 108
DakotaModel, 129
HierLayeredModel, 239
NestedModel, 270
SingleModel, 334
SurrLayeredModel, 356
totalPatternSize
DataMethod, 193
toUpper
DakotaString, 165
transNataf
NonDAdvMeanValue, 284
transUToX
NonDAdvMeanValue, 278, 282
transUToZ
NonDAdvMeanValue, 283
transXToU
NonDAdvMeanValue, 282
transXToZ
NonDAdvMeanValue, 282
transZToU
NonDAdvMeanValue, 283
trRatioContractValue
SurrBasedOptStrategy, 351
trRatioExpandValue
SurrBasedOptStrategy, 351
trustRegionFactor
SurrBasedOptStrategy, 351
trustRegionSize
SurrBasedOptStrategy, 351
tv
AllMergedVariables, 28
AllVariables, 35
DakotaModel, 130
DakotaVariables, 174
FundamentalVariables, 227
MergedVariables, 262

uncertain
DataVariables, 203
uncertainCorrelations
DakotaNonD, 140
DataVariables, 206
uncertainDistLowerBnds
DataVariables, 206
FundamentalVarConstraints, 225
MergedVarConstraints, 261
uncertainDistUpperBnds
DataVariables, 206
FundamentalVarConstraints, 225
MergedVarConstraints, 261
uncertainLabels
DataVariables, 206
FundamentalVariables, 230
MergedVariables, 264
uncertainVars
DataVariables, 206
FundamentalVariables, 229
MergedVariables, 264
uniformDistLowerBnds

DakotaNonD, 140
uniformDistUpperBnds
DakotaNonD, 140
uniformUncDistLowerBnds
DataVariables, 205
uniformUncDistUpperBnds
DataVariables, 205
unixCommand
CommandShell, 68
update_all_continuous
VariablesUtil, 368
update_all_discrete
VariablesUtil, 368
update_approximation
ApproximationInterface, 55
DakotaInterface, 108
DakotaModel, 128
SurrLayeredModel, 356
update_best
DACEIterator, 81
DakotaIterator, 114
ParamStudy, 313
update_labels
VariablesUtil, 368
update_merged
VariablesUtil, 367
update_response
DakotaModel, 138
upper
DakotaString, 166
upperBounds
NPSOLOptimizer, 295
upperFactorHessianF77
SOLBase, 348
usage
GetLongOpt, 232, 234
user_defined_model
DakotaIterator, 114
userConstraintEval
NPSOLOptimizer, 295
userDefinedInterface
SingleModel, 334
userDefinedModel
BranchBndStrategy, 59
COLINApplication, 61
ConcurrentStrategy, 70
DakotaIterator, 115
SGOPTApplication, 325
SingleMethodStrategy, 331
userDefinedModels
MultilevelOptStrategy, 267
userDefinedVarConstraints
DakotaModel, 133
userObjectiveEval
NPSOLOptimizer, 295
ustring
GetLongOpt, 233

varConstraintsRep
DakotaVarConstraints, 171
variablePartitions
ParamStudy, 314
variables_kwhandler
ProblemDescDB, 318
variables_type
DakotaVariables, 176
variablesIter
ProblemDescDB, 319
variablesList
ProblemDescDB, 319
variablesPointer
DataMethod, 189
variablesRep
DakotaVariables, 177
variablesType
DakotaVarConstraints, 170
DakotaVariables, 176
VariablesUtil
~VariablesUtil, 367
update_all_continuous, 368
update_all_discrete, 368
update_labels, 368
update_merged, 367
VariablesUtil, 367
VariablesUtil, 367
varPartitions
DataMethod, 193
varsList
DakotaModel, 135
varyPattern
DACEIterator, 82
NonDSampling, 292
vector_loop
ParamStudy, 312
vendorNumericalGradFlag
DakotaOptLeastSq, 148
verboseFlag
AnalysisCode, 40
DakotaApproximation, 86
DakotaInterface, 110
verboseOutput
DakotaIterator, 116
verifyLevel
DataMethod, 191

waitall
ParallelLibrary, 299
weibullAlphas

DakotaNonD, 140
weibullBetas
DakotaNonD, 140
weibullUncAlphas
DataVariables, 206
weibullUncBetas
DataVariables, 206
win2dOn
DakotaGraphics, 104
win3dOn
DakotaGraphics, 104
workVector
KrigApprox, 246
workVectorQuad
KrigApprox, 246
world_rank
DakotaStrategy, 159
ParallelLibrary, 299
world_size
ParallelLibrary, 299
worldRank
ApplicationInterface, 46
DakotaStrategy, 160
ParallelLibrary, 302
worldSize
ApplicationInterface, 46
DakotaStrategy, 160
ParallelLibrary, 302
write
AllMergedVarConstraints, 26
AllMergedVariables, 29, 30
AllVarConstraints, 33
AllVariables, 36, 37
DakotaResponse, 151
DakotaResponseRep, 157, 158
DakotaVarConstraints, 169
DakotaVariables, 176
DataInterface, 184
DataMethod, 189
DataResponses, 196
DataStrategy, 199
DataVariables, 203
FundamentalVarConstraints, 224
FundamentalVariables, 228, 229
MergedVarConstraints, 260
MergedVariables, 263, 264
ParamResponsePair, 309, 310
write_annotated
AllMergedVariables, 29
AllVariables, 36
DakotaResponse, 151
DakotaResponseRep, 157
DakotaVariables, 176
FundamentalVariables, 229
MergedVariables, 263
ParamResponsePair, 309
write_data
DakotaResponse, 152
DakotaResponseRep, 155
write_parameters_file
AnalysisCode, 39
write_precision
main.C, 370
restart_util.C, 371
write_tabular
DakotaResponse, 151
DakotaResponseRep, 157
DakotaVariables, 176
ParamResponsePair, 309

x_matrix
KrigingSurf, 250
xdrInBuf
DakotaBiStream, 99
xdrOutBuf
DakotaBoStream, 102
xMatrix
KrigApprox, 245
xNewVector
KrigApprox, 245
xVect
DirectFnApplicInterface, 209

yfbRinvVector
KrigApprox, 246
yfbVector
KrigApprox, 246
yNewVector
KrigApprox, 245
yValueVector
KrigApprox, 245