Calibrator

1.2.1

Generated by Doxygen 1.8.9.1

Fri Nov 27 2015 08:04:37

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Chapter 1

MPCOTool

The Multi-Purposes Calibration and Optimization Tool. A software to perform calibrations or optimizations of empirical parameters.

VERSIONS

- 1.2.1: Stable and recommended version.
- 1.3.7: Developing version to do new features.

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TOOLS AND LIBRARIES REQUIRED TO BUILD THE EXECUTABLE

- gcc or clang (to compile the source code)
- make (to build the executable file)
- autoconf (to generate the Makefile in different operative systems)
- automake (to check the operative system)
- pkg-config (to find the libraries to compile)
- gsl (to generate random numbers)
- libxml (to deal with XML files)
- glib (extended utilities of C to work with data, lists, mapped files, regular expressions, using multicores in shared memory machines, ...)
- genetic (genetic algorithm)

OPTIONAL TOOLS AND LIBRARIES

- gettext (to work with different locales)
- gtk+ (to create the interactive GUI tool)
- openmpi or mpich (to run in parallelized tasks on multiple computers)

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- doxygen (standard comments format to generate documentation)
- latex (to build the PDF manuals)

FILES

The source code has to have the following files:

- 1.2.1/configure.ac: configure generator.
- 1.2.1/Makefile.in: Makefile generator.
- 1.2.1/config.h.in: config header generator.
- 1.2.1/mpcotool.c: main source code.
- 1.2.1/mpcotool.h: main header code.
- 1.2.1/interface.h: interface header code.
- 1.2.1/build: script to build all.
- 1.2.1/logo.png: logo figure.
- 1.2.1/Doxyfile: configuration file to generate doxygen documentation.
- · TODO: tasks to do.
- · README.md: this file.
- tests/testX/*: several tests to check the program working.
- locales/*/LC_MESSAGES/mpcotool.po: translation files.
- manuals/*.eps: manual figures in EPS format.
- manuals/*.png: manual figures in PNG format.
- manuals/*.tex: documentation source files.
- applications/*/*: several practical application cases.
- check_errors/*.xml: several mistaken files to check error handling.

BUILDING INSTRUCTIONS

This software has been built and tested in the following operative systems. Probably, it can be built in other systems, distributions, or versions but it has not been tested.

Debian 8 (Linux, kFreeBSD or Hurd)

DragonFly BSD 4.2

Dyson Illumos

FreeBSD 10.2

Linux Mint DE 2

NetBSD 7.0

OpenSUSE Linux 13

Ubuntu Linux 12, 14, and 15

1. Download the latest genetic doing on a terminal:

```
$ git clone https://github.com/jburguete/genetic.git
```

2. Download this repository:

```
$ git clone https://github.com/jburguete/mpcotool.git
```

3. Link the latest genetic version to genetic:

```
$ cd mpcotool/1.2.1
$ In -s ../../genetic/0.6.1 genetic
```

4. Build doing on a terminal:

\$./build

OpenBSD 5.8

1. Select adequate versions:

```
$ export AUTOCONF_VERSION=2.69 AUTOMAKE_VERSION=1.15
```

2. Then, in a terminal, follow steps 1 to 4 of the previous Debian 8 section.

Microsoft Windows 7 (with MSYS2)

Microsoft Windows 8.1 (with MSYS2)

- 1. Install MSYS2 and the required libraries and utilities. You can follow detailed instructions in install-unix
- 2. Then, in a MSYS2 terminal, follow steps 1 to 4 of the previous Debian 8 section.
- 3. Optional Windows binary package can be built doing in the terminal:

\$ make windist

Fedora Linux 23

1. In order to use OpenMPI compilation do in a terminal (in 64 bits version):

```
$ export PATH=$PATH:/usr/lib64/openmpi/bin
```

2. Then, follow steps 1 to 4 of the previous Debian 8 section.

MAKING MANUALS INSTRUCTIONS

On UNIX type systems you need texlive installed. On Windows systems you need MiKTeX. In order to compile the manuals you can type on a terminal:

\$ make manuals

MAKING TESTS INSTRUCTIONS

In order to build the tests follow the next instructions:

1. Link some tests that needs genetic library doing in a terminal (assuming that you are in the directory mpcotool/1.2.1):

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```
$ cd ../tests/test2
```

\$ In -s ../../genetic/0.6.1 genetic

\$ cd ../test3

\$ In -s ../../genetic/0.6.1 genetic

\$ cd ../test4

\$ In -s ../../genetic/0.6.1 genetic

2. Build all tests doing in the same terminal:

\$ cd ../../1.2.1

\$ make tests

USER INSTRUCTIONS

- · Command line in sequential mode:
 - \$./mpcotoolbin [-nthreads X] input_file.xml
- · Command line in parallelized mode (where X is the number of threads to open in every node):
 - \$ mpirun [MPI options] ./mpcotoolbin [-nthreads X] input file.xml
- · The syntax of the simulator has to be:
 - \$./simulator name input file 1 [input file 2] [input file 3] [input file 4] output file
- The syntax of the program to evaluate the objetive function has to be (where the first data in the results file has to be the objective function value):
 - \$./evaluator_name simulated_file data_file results_file
- On UNIX type systems the GUI application can be open doing on a terminal:
 - \$./mpcotool

INPUT FILE FORMAT

The format of the main input file is as:

"xml <?xml version="1.0"?> <calibrate simulator="simulator_name" evaluator="evaluator_name" algorithm="algorithm="type" nsimulations="simulations_number" niterations="iterations_number" tolerance="tolerance_value" nbest="best in __number" npopulation="population_number" ngenerations="generations_number" mutation="mutation_index adaptation="adaptation_ratio" gradient_type="gradient_method_type" nsteps="steps_number" relaxation="relaxation_paramter" nestimates="estimates_number" seed="random_index seed" result="result_file" variables="variables_file"> <experiment name="data_file_1" template1="template_1_1" template2="template_1_2" ... weight="weight_1"/> ... <experiment name="data_file_N" template1="template" __n_1" template2="template_N_2" ... weight="weight_N"/> <variable name="variable_1" minimum="min_value" maximum="max_value" precision="precision_digits" sweeps="sweeps_number" nbits="bits_number" step="step_index of the precision in _ precision _ digits" sweeps="sweeps_number" nbits="bits_number" step="step_size"> </calibrate> ""

with:

- simulator: simulator executable file name.
- evaluator: Optional. When needed is the evaluator executable file name.
- seed: Optional. Seed of the pseudo-random numbers generator (default value is 7007).
- result: Optional. It is the name of the optime result file (default name is "result").
- variables: Optional. It is the name of all simulated variables file (default name is "variables").

- **precision**: Optional, defined for each variable. Number of precision digits to evaluate the variable. 0 apply for integer numbers (default value is 14).
- weight Optional, defined for each experiment. Multiplies the objective value obtained for each experiment in the final objective function value (default value is 1).

Implemented algorithms are:

- sweep: Sweep brute force algorithm. It requires for each variable:
 - sweeps: number of sweeps to generate for each variable in every experiment.

The total number of simulations to run is:

(number of experiments) x (variable 1 number of sweeps) x ... x (variable n number of sweeps) x (number of iterations)

- Monte-Carlo: Monte-Carlo brute force algorithm. It requires on calibrate:
 - nsimulations: number of simulations to run in every experiment.

The total number of simulations to run is:

(number of experiments) x (number of simulations) x (number of iterations)

- Both brute force algorithms can be iterated to improve convergence by using the following parameters:
 - nbest: number of best simulations to calculate convergence interval on next iteration (default 1).
 - tolerance: tolerance parameter to increase convergence interval (default 0).
 - niterations: number of iterations (default 1).

It multiplies the total number of simulations:

x (number of iterations)

- · Moreover, both brute force algorithms can be coupled with a gradient based method by using:
 - gradient_type: method to estimate the gradient. Two options are currently available:
 - * coordinates: coordinates descent method.

It increases the total number of simulations by:

(number of experiments) x (number of iterations) x (number of steps) x 2 x (number of variables)

- * random: random method. It requires:
- * nestimates: number of random checks to estimate the gradient.

It increases the total number of simulations by:

(number of experiments) x (number of iterations) x (number of steps) x (number of estimates)

Both methods require also:

- nsteps: number of steps to perform the gradient based method,
- relaxation: relaxation parameter,

and for each variable:

- step: initial step size for the gradient based method.
- genetic: Genetic algorithm. It requires the following parameters:
 - npopulation: number of population.
 - ngenerations: number of generations.
 - mutation: mutation ratio.
 - reproduction: reproduction ratio.
 - adaptation: adaptation ratio.

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and for each variable:

- nbits: number of bits to encode each variable.

The total number of simulations to run is:

```
(number of experiments) x (npopulation) x [1 + (ngenerations - 1) x (mutation + reproduction + adaptation)]
```

SOME EXAMPLES OF INPUT FILES

Example 1

- The simulator program name is: pivot
- · The syntax is:

```
$ ./pivot input_file output_file
```

- The program to evaluate the objective function is: compare
- · The syntax is:
 - \$./compare simulated file data file result file
- The calibration is performed with a sweep brute force algorithm.
- The experimental data files are:

```
27-48.txt
42.txt
52.txt
100.txt
```

• Templates to get input files to simulator for each experiment are:

```
template1.js
template2.js
template3.js
template4.js
```

• The variables to calibrate, ranges, precision and sweeps number to perform are:

```
alpha1, [179.70, 180.20], 2, 5
alpha2, [179.30, 179.60], 2, 5
random, [0.00, 0.20], 2, 5
boot-time, [0.0, 3.0], 1, 5
```

- Then, the number of simulations to run is: 4x5x5x5x5=2500.
- · The input file is:

• A template file as template1.js:

```
"` { "towers" : [ { "length" : 50.11, "velocity" : 0.02738, "@variable1@" : @, "@variable2@" : @, "@variable3@" : @, "@variable4@" : @ }, { "length" : 50.11, "velocity" : 0.02824, "@variable1@" : @, "@variable2@" : @, "@variable3@" : @, "@variable4@" : @ }, { "length" : 50.11, "velocity" : 0.03008, "@variable1@" : @, "@variable2@" : @, "@variable3@" : @, "@variable4@" : @ }, { "length" : 50.11, "velocity" : 0.03753, "@variable1@" : @, "@variable2@" : @, "@variable2@" : @, "@variable3@" : @, "@variable4@" : @ } ], "cycle-time" : 71.0, "plot-time" : 1.0, "comp-time-step": 0.1, "active-percent" : 27.48 } "
```

• produces simulator input files to reproduce the experimental data file 27-48.txt as:

```
 \begin{tabular}{ll} \be
```

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Chapter 2

Data Structure Index

2.1 Data Structures

Here are the data structures with brief descriptions:

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Chapter 3

File Index

3.1 File List

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

ontig.h
Configuration header file
nterface.h
Header file of the interface
npcotool.c
Source file of the mpcotool
npcotool.h
Header file of the mpcotool

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Chapter 4

Data Structure Documentation

4.1 Calibrate Struct Reference

Struct to define the calibration data.

```
#include <mpcotool.h>
```

Data Fields

• GMappedFile ** file [MAX_NINPUTS]

Matrix of input template files.

char ** template [MAX_NINPUTS]

Matrix of template names of input files.

• char ** experiment

Array of experimental data file names.

char ** label

Array of variable names.

• gsl_rng * rng

GSL random number generator.

• GeneticVariable * genetic_variable

Array of variables for the genetic algorithm.

• FILE * file_result

Result file.

• FILE * file_variables

Variables file.

• char * result

Name of the result file.

• char * variables

Name of the variables file.

• char * simulator

Name of the simulator program.

• char * evaluator

Name of the program to evaluate the objective function.

• double * value

Array of variable values.

• double * rangemin

Array of minimum variable values.

double * rangemax

Array of maximum variable values.

• double * rangeminabs

Array of absolute minimum variable values.

• double * rangemaxabs

Array of absolute maximum variable values.

double * error_best

Array of the best minimum errors.

double * weight

Array of the experiment weights.

double * step

Array of gradient based method step sizes.

double * gradient

Vector of gradient estimation.

double * value_old

Array of the best variable values on the previous step.

double * error old

Array of the best minimum errors on the previous step.

• unsigned int * precision

Array of variable precisions.

• unsigned int * nsweeps

Array of sweeps of the sweep algorithm.

• unsigned int * thread

Array of simulation numbers to calculate on the thread.

- unsigned int * thread_gradient
- unsigned int * simulation_best

Array of best simulation numbers.

· double tolerance

Algorithm tolerance.

• double mutation_ratio

Mutation probability.

• double reproduction_ratio

Reproduction probability.

double adaptation_ratio

Adaptation probability.

· double relaxation

Relaxation parameter.

double calculation_time

Calculation time.

· unsigned long int seed

Seed of the pseudo-random numbers generator.

• unsigned int nvariables

Variables number.

unsigned int nexperiments

Experiments number.

· unsigned int ninputs

Number of input files to the simulator.

· unsigned int nsimulations

Simulations number per experiment.

· unsigned int gradient_method

Method to estimate the gradient.

unsigned int nsteps

Number of steps for the gradient based method.

• unsigned int nestimates

Number of simulations to estimate the gradient.

· unsigned int algorithm

Algorithm type.

· unsigned int nstart

Beginning simulation number of the task.

· unsigned int nend

Ending simulation number of the task.

· unsigned int nstart_gradient

Beginning simulation number of the task for the gradient based method.

unsigned int nend_gradient

Ending simulation number of the task for the gradient based method.

· unsigned int niterations

Number of algorithm iterations.

· unsigned int nbest

Number of best simulations.

· unsigned int nsaveds

Number of saved simulations.

int mpi_rank

Number of MPI task.

4.1.1 Detailed Description

Struct to define the calibration data.

Definition at line 111 of file mpcotool.h.

4.1.2 Field Documentation

4.1.2.1 unsigned int* Calibrate::thread_gradient

Array of simulation numbers to calculate on the thread for the gradient based method.

Definition at line 144 of file mpcotool.h.

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

· mpcotool.h

4.2 Experiment Struct Reference

Struct to define experiment data.

```
#include <interface.h>
```

Data Fields

char * template [MAX_NINPUTS]

Array of input template names.

• char * name

File name.

· double weight

Weight to calculate the objective function value.

4.2.1 Detailed Description

Struct to define experiment data.

Definition at line 46 of file interface.h.

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

· interface.h

4.3 Input Struct Reference

Struct to define the calibration input file.

```
#include <mpcotool.h>
```

Data Fields

char ** template [MAX_NINPUTS]

Matrix of template names of input files.

char ** experiment

Array of experimental data file names.

• char ** label

Array of variable names.

· char * result

Name of the result file.

char * variables

Name of the variables file.

char * simulator

Name of the simulator program.

• char * evaluator

Name of the program to evaluate the objective function.

char * directory

Working directory.

• char * name

Input data file name.

• double * rangemin

Array of minimum variable values.

• double * rangemax

Array of maximum variable values.

• double * rangeminabs

Array of absolute minimum variable values.

• double * rangemaxabs

Array of absolute maximum variable values.

double * weight

Array of the experiment weights.

double * step

Array of gradient based method step sizes.

• unsigned int * precision

Array of variable precisions.

• unsigned int * nsweeps

Array of sweeps of the sweep algorithm.

• unsigned int * nbits

Array of bits numbers of the genetic algorithm.

· double tolerance

Algorithm tolerance.

• double mutation_ratio

Mutation probability.

· double reproduction_ratio

Reproduction probability.

· double adaptation ratio

Adaptation probability.

· double relaxation

Relaxation parameter.

· unsigned long int seed

Seed of the pseudo-random numbers generator.

· unsigned int nvariables

Variables number.

· unsigned int nexperiments

Experiments number.

· unsigned int ninputs

Number of input files to the simulator.

• unsigned int nsimulations

Simulations number per experiment.

· unsigned int algorithm

Algorithm type.

unsigned int nsteps

Number of steps to do the gradient based method.

· unsigned int gradient_method

Method to estimate the gradient.

• unsigned int nestimates

Number of simulations to estimate the gradient.

· unsigned int niterations

Number of algorithm iterations.

· unsigned int nbest

Number of best simulations.

4.3.1 Detailed Description

Struct to define the calibration input file.

Definition at line 64 of file mpcotool.h.

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

· mpcotool.h

4.4 Options Struct Reference

Struct to define the options dialog.

#include <interface.h>

Data Fields

• GtkDialog * dialog

Main GtkDialog.

• GtkGrid * grid

Main GtkGrid.

• GtkLabel * label_seed

Pseudo-random numbers generator seed GtkLabel.

• GtkSpinButton * spin_seed

Pseudo-random numbers generator seed GtkSpinButton.

• GtkLabel * label_threads

Threads number GtkLabel.

• GtkSpinButton * spin_threads

Threads number GtkSpinButton.

• GtkLabel * label_gradient

Gradient threads number GtkLabel.

• GtkSpinButton * spin_gradient

Gradient threads number GtkSpinButton.

4.4.1 Detailed Description

Struct to define the options dialog.

Definition at line 74 of file interface.h.

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

· interface.h

4.5 ParallelData Struct Reference

Struct to pass to the GThreads parallelized function.

```
#include <mpcotool.h>
```

Data Fields

· unsigned int thread

Thread number.

4.5.1 Detailed Description

Struct to pass to the GThreads parallelized function.

Definition at line 184 of file mpcotool.h.

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

mpcotool.h

4.6 Running Struct Reference

Struct to define the running dialog.

```
#include <interface.h>
```

Data Fields

• GtkDialog * dialog

Main GtkDialog.

• GtkLabel * label

Label GtkLabel.

4.6.1 Detailed Description

Struct to define the running dialog.

Definition at line 92 of file interface.h.

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

· interface.h

4.7 Variable Struct Reference

Struct to define variable data.

```
#include <interface.h>
```

Data Fields

• char * label

Variable label.

• double rangemin

Minimum value.

• double rangemax

Maximum value.

· double rangeminabs

Minimum allowed value.

• double rangemaxabs

Maximum allowed value.

· unsigned int precision

Precision digits.

• unsigned int nsweeps

Sweeps number of the sweep algorithm.

· unsigned int nbits

Bits number of the genetic algorithm.

4.7.1 Detailed Description

Struct to define variable data.

Definition at line 58 of file interface.h.

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

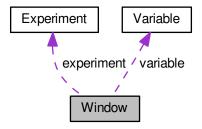
· interface.h

4.8 Window Struct Reference

Struct to define the main window.

#include <interface.h>

Collaboration diagram for Window:



Data Fields

• GtkWindow * window

Main GtkWindow.

• GtkGrid * grid

Main GtkGrid.

GtkToolbar * bar buttons

GtkToolbar to store the main buttons.

• GtkToolButton * button_open

Open GtkToolButton.

• GtkToolButton * button_save

Save GtkToolButton.

GtkToolButton * button_run

Run GtkToolButton.

• GtkToolButton * button options

Options GtkToolButton.

GtkToolButton * button_help

Help GtkToolButton.

• GtkToolButton * button_about

Help GtkToolButton.

GtkToolButton * button_exit

Exit GtkToolButton.

GtkGrid * grid_files

Files GtkGrid.

• GtkLabel * label_simulator

Simulator program GtkLabel.

• GtkFileChooserButton * button simulator

Simulator program GtkFileChooserButton.

GtkCheckButton * check evaluator

Evaluator program GtkCheckButton.

• GtkFileChooserButton * button_evaluator

Evaluator program GtkFileChooserButton.

• GtkLabel * label result

Result file GtkLabel.

• GtkEntry * entry_result

Result file GtkEntry.

• GtkLabel * label variables

Variables file GtkLabel.

• GtkEntry * entry_variables

Variables file GtkEntry.

GtkFrame * frame algorithm

GtkFrame to set the algorithm.

• GtkGrid * grid_algorithm

GtkGrid to set the algorithm.

GtkRadioButton * button_algorithm [NALGORITHMS]

Array of GtkButtons to set the algorithm.

• GtkLabel * label simulations

GtkLabel to set the simulations number.

• GtkSpinButton * spin_simulations

GtkSpinButton to set the simulations number.

• GtkLabel * label iterations

GtkLabel to set the iterations number.

GtkSpinButton * spin_iterations

GtkSpinButton to set the iterations number.

• GtkLabel * label_tolerance

GtkLabel to set the tolerance.

• GtkSpinButton * spin_tolerance

GtkSpinButton to set the tolerance.

• GtkLabel * label_bests

GtkLabel to set the best number.

GtkSpinButton * spin_bests

GtkSpinButton to set the best number.

• GtkLabel * label population

GtkLabel to set the population number.

GtkSpinButton * spin_population

GtkSpinButton to set the population number.

• GtkLabel * label_generations

GtkLabel to set the generations number.

GtkSpinButton * spin_generations

GtkSpinButton to set the generations number.

• GtkLabel * label_mutation

GtkLabel to set the mutation ratio.

• GtkSpinButton * spin_mutation

GtkSpinButton to set the mutation ratio.

• GtkLabel * label_reproduction

GtkLabel to set the reproduction ratio.

GtkSpinButton * spin_reproduction

GtkSpinButton to set the reproduction ratio.

• GtkLabel * label adaptation

GtkLabel to set the adaptation ratio.

• GtkSpinButton * spin_adaptation

GtkSpinButton to set the adaptation ratio.

GtkCheckButton * check gradient

GtkCheckButton to check running the gradient based method.

GtkGrid * grid_gradient

GtkGrid to pack the gradient based method widgets.

GtkRadioButton * button gradient [NGRADIENTS]

GtkRadioButtons array to set the gradient estimate method.

GtkLabel * label_steps

GtkLabel to set the steps number.

• GtkSpinButton * spin_steps

GtkSpinButton to set the steps number.

• GtkLabel * label estimates

GtkLabel to set the estimates number.

• GtkSpinButton * spin_estimates

GtkSpinButton to set the estimates number.

• GtkLabel * label_relaxation

GtkLabel to set the relaxation parameter.

GtkSpinButton * spin_relaxation

GtkSpinButton to set the relaxation parameter.

• GtkFrame * frame_variable

Variable GtkFrame.

• GtkGrid * grid_variable

Variable GtkGrid.

• GtkComboBoxText * combo_variable

GtkComboBoxEntry to select a variable.

• GtkButton * button add variable

GtkButton to add a variable.

GtkButton * button_remove_variable

GtkButton to remove a variable.

• GtkLabel * label variable

Variable GtkLabel.

GtkEntry * entry variable

GtkEntry to set the variable name.

• GtkLabel * label_min

Minimum GtkLabel.

• GtkSpinButton * spin min

Minimum GtkSpinButton.

• GtkScrolledWindow * scrolled min

Minimum GtkScrolledWindow.

GtkLabel * label max

Maximum GtkLabel.

• GtkSpinButton * spin_max

Maximum GtkSpinButton.

GtkScrolledWindow * scrolled_max

Maximum GtkScrolledWindow.

GtkCheckButton * check minabs

Absolute minimum GtkCheckButton.

GtkSpinButton * spin minabs

Absolute minimum GtkSpinButton.

GtkScrolledWindow * scrolled minabs

Absolute minimum GtkScrolledWindow.

GtkCheckButton * check_maxabs

Absolute maximum GtkCheckButton.

GtkSpinButton * spin_maxabs

Absolute maximum GtkSpinButton.

• GtkScrolledWindow * scrolled_maxabs

Absolute maximum GtkScrolledWindow.

• GtkLabel * label_precision

Precision GtkLabel.

• GtkSpinButton * spin_precision

Precision digits GtkSpinButton.

GtkLabel * label sweeps

Sweeps number GtkLabel.

• GtkSpinButton * spin_sweeps

Sweeps number GtkSpinButton.

GtkLabel * label_bits

Bits number GtkLabel.

• GtkSpinButton * spin_bits

Bits number GtkSpinButton.

GtkFrame * frame_experiment

Experiment GtkFrame.

GtkGrid * grid experiment

Experiment GtkGrid.

• GtkComboBoxText * combo_experiment

Experiment GtkComboBoxEntry.

• GtkButton * button_add_experiment

GtkButton to add a experiment.

• GtkButton * button_remove_experiment

GtkButton to remove a experiment.

• GtkLabel * label_experiment

Experiment GtkLabel.

GtkFileChooserButton * button_experiment

GtkFileChooserButton to set the experimental data file.

• GtkLabel * label weight

Weight GtkLabel.

GtkSpinButton * spin_weight

Weight GtkSpinButton.

GtkCheckButton * check_template [MAX_NINPUTS]

Array of GtkCheckButtons to set the input templates.

GtkFileChooserButton * button_template [MAX_NINPUTS]

Array of GtkFileChooserButtons to set the input templates.

• GdkPixbuf * logo

Logo GdkPixbuf.

• Experiment * experiment

Array of experiments data.

• Variable * variable

Array of variables data.

• char * application_directory

Application directory.

• gulong id_experiment

Identifier of the combo_experiment signal.

• gulong id_experiment_name

Identifier of the button_experiment signal.

• gulong id_variable

Identifier of the combo_variable signal.

• gulong id_variable_label

Identifier of the entry_variable signal.

• gulong id_template [MAX_NINPUTS]

Array of identifiers of the check_template signal.

• gulong id_input [MAX_NINPUTS]

Array of identifiers of the button_template signal.

• unsigned int nexperiments

Number of experiments.

· unsigned int nvariables

Number of variables.

4.8.1 Detailed Description

Struct to define the main window.

Definition at line 102 of file interface.h.

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

• interface.h

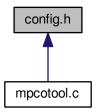
Chapter 5

File Documentation

5.1 config.h File Reference

Configuration header file.

This graph shows which files directly or indirectly include this file:



Macros

#define MAX_NINPUTS 8

Maximum number of input files in the simulator program.

• #define NALGORITHMS 3

Number of stochastic algorithms.

• #define NGRADIENTS 2

Number of gradient estimate methods.

• #define NPRECISIONS 15

Number of precisions.

• #define DEFAULT_PRECISION (NPRECISIONS - 1)

Default precision digits.

• #define DEFAULT_RANDOM_SEED 7007

Default pseudo-random numbers seed.

#define DEFAULT_RELAXATION 1.

Default relaxation parameter.

• #define LOCALE_DIR "locales"

Locales directory.

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 #define PROGRAM_INTERFACE "mpcotool" Name of the interface program. • #define XML ABSOLUTE MINIMUM (const xmlChar*)"absolute minimum" absolute minimum XML label. #define XML_ABSOLUTE_MAXIMUM (const xmlChar*)"absolute_maximum" absolute maximum XML label. • #define XML ADAPTATION (const xmlChar*)"adaptation" adaption XML label. #define XML_ALGORITHM (const xmlChar*)"algorithm" algoritm XML label. #define XML CALIBRATE (const xmlChar*)"calibrate" calibrate XML label. #define XML_COORDINATES (const xmlChar*)"coordinates" coordinates XML label. #define XML EVALUATOR (const xmlChar*)"evaluator" evaluator XML label. #define XML_EXPERIMENT (const xmlChar*)"experiment" experiment XML label. • #define XML_GENETIC (const xmlChar*)"genetic" genetic XML label. #define XML_GRADIENT_METHOD (const xmlChar*)"gradient_method" gradient_method XML label. #define XML_MINIMUM (const xmlChar*)"minimum" minimum XML label. #define XML_MAXIMUM (const xmlChar*)"maximum" maximum XML label. #define XML MONTE CARLO (const xmlChar*)"Monte-Carlo" Monte-Carlo XML label. • #define XML_MUTATION (const xmlChar*)"mutation" mutation XML label. #define XML_NAME (const xmlChar*)"name" name XML label. #define XML_NBEST (const xmlChar*)"nbest" nbest XML label. #define XML NBITS (const xmlChar*)"nbits" nbits XML label. #define XML NESTIMATES (const xmlChar*)"nestimates" nestimates XML label. #define XML_NGENERATIONS (const xmlChar*)"ngenerations" ngenerations XML label. • #define XML NITERATIONS (const xmlChar*)"niterations" niterations XML label. #define XML_NPOPULATION (const xmlChar*)"npopulation" npopulation XML label. • #define XML NSIMULATIONS (const xmlChar*)"nsimulations" nsimulations XML label. • #define XML_NSTEPS (const xmlChar*)"nsteps" nsteps XML label. #define XML NSWEEPS (const xmlChar*)"nsweeps"

nsweeps XML label.

#define XML_PRECISION (const xmlChar*)"precision"

precision XML label.

 #define XML_RANDOM (const xmlChar*)"random" random XML label.

 #define XML_RELAXATION (const xmlChar*)"relaxation" relaxation XML label.

 #define XML_REPRODUCTION (const xmlChar*)"reproduction" reproduction XML label.

 #define XML_RESULT (const xmlChar*)"result" result XML label.

 #define XML_SIMULATOR (const xmlChar*)"simulator" simulator XML label.

 #define XML_SEED (const xmlChar*)"seed" seed XML label.

 #define XML_STEP (const xmlChar*)"step" step XML label.

 #define XML_SWEEP (const xmlChar*)"sweep" sweep XML label.

 #define XML_TEMPLATE1 (const xmlChar*)"template1" template1 XML label.

 #define XML_TEMPLATE2 (const xmlChar*)"template2" template2 XML label.

 #define XML_TEMPLATE3 (const xmlChar*)"template3" template3 XML label.

 #define XML_TEMPLATE4 (const xmlChar*)"template4" template4 XML label.

 #define XML_TEMPLATE5 (const xmlChar*)"template5" template5 XML label.

 #define XML_TEMPLATE6 (const xmlChar*)"template6" template6 XML label.

 #define XML_TEMPLATE7 (const xmlChar*)"template7" template7 XML label.

 #define XML_TEMPLATE8 (const xmlChar*)"template8" template8 XML label.

 #define XML_TOLERANCE (const xmlChar*)"tolerance" tolerance XML label.

 #define XML_VARIABLE (const xmlChar*)"variable" variable XML label.

 #define XML_VARIABLES (const xmlChar*)"variables" variables XML label.

 #define XML_WEIGHT (const xmlChar*)"weight" weight XML label.

5.1.1 Detailed Description

Configuration header file.

Authors

Javier Burguete and Borja Latorre.

Copyright

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Definition in file config.h.

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5.2 config.h

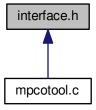
```
00001 /* config.h. Generated from config.h.in by configure. \star/
00003 MPCOTool: a software to make calibrations of empirical parameters.
00004
00005 AUTHORS: Javier Burguete and Borja Latorre.
00006
00007 Copyright 2012-2014, AUTHORS.
00008
00009 Redistribution and use in source and binary forms, with or without modification,
00010 are permitted provided that the following conditions are met:
00012
           1. Redistributions of source code must retain the above copyright notice,
00013
               this list of conditions and the following disclaimer.
00014
           2. Redistributions in binary form must reproduce the above copyright notice,
00016
               this list of conditions and the following disclaimer in the
00017
               documentation and/or other materials provided with the distribution.
00018
00019 THIS SOFTWARE IS PROVIDED BY AUTHORS ''AS IS'' AND ANY EXPRESS OR IMPLIED 00020 WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF 00021 MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT
00022 SHALL AUTHORS OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL,
00023 SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO,
00024 PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR
00025 BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN
00026 CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING
00027 IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY
00028 OF SUCH DAMAGE.
00029 */
00030
00037 #ifndef CONFIG__H
00038 #define CONFIG_H 1
00039
00040 // Array sizes
00041
00042 #define MAX_NINPUTS 8
00043 #define NALGORITHMS 3
00045 #define NGRADIENTS 2
00046 #define NPRECISIONS 15
00047
00048 // Default choices
00049
00050 #define DEFAULT_PRECISION (NPRECISIONS - 1)
00051 #define DEFAULT_RANDOM_SEED 7007
00052 #define DEFAULT_RELAXATION 1.
00054 // Interface labels
00055
00056 #define LOCALE_DIR "locales" 00057 #define PROGRAM_INTERFACE "mpcotool"
00058
00059 // XML labels
00060
00061 #define XML_ABSOLUTE_MINIMUM (const xmlChar*)"absolute_minimum"
00062 #define XML_ABSOLUTE_MAXIMUM (const xmlChar*) "absolute_maximum"
00064 #define XML_ADAPTATION (const xmlChar*)"adaptation"
00066 #define XML_ALGORITHM (const xmlChar*) "algorithm"
00068 #define XML_CALIBRATE (const xmlChar*)"calibrate"
00070 #define XML_COORDINATES (const xmlChar*)"coordinates"
00072 #define XML_EVALUATOR (const xmlChar*)"evaluator"
00074 #define XML_EXPERIMENT (const xmlChar*)"experiment"
00076 #define XML_GENETIC (const xmlChar*)"genetic"
00078 #define XML_GRADIENT_METHOD (const xmlChar*)"gradient_method"
00079 #define XML_MINIMUM (const xmlChar*) "minimum"
00081 #define XML_MAXIMUM (const xmlChar*)"maximum"
00082 #define XML_MONTE_CARLO (const xmlChar*)"Monte-Carlo"
00083 #define XML_MUTATION (const xmlChar*) "mutation"
00085 #define XML_NAME (const xmlChar*)"name" 00086 #define XML_NBEST (const xmlChar*)"nbest"
00087 #define XML_NBITS (const xmlChar*) "nbits"
00088 #define XML_NESTIMATES (const xmlChar*) "nestimates"
00089 #define XML_NGENERATIONS (const xmlChar*)"ngenerations"
00091 #define XML_NITERATIONS (const xmlChar*)"niterations" 00093 #define XML_NPOPULATION (const xmlChar*)"npopulation"
00095 #define XML_NSIMULATIONS (const xmlChar*) "nsimulations" 00097 #define XML_NSTEPS (const xmlChar*) "nsteps"
00099 #define XML_NSWEEPS (const xmlChar*) "nsweeps"
00100 #define XML_PRECISION (const xmlChar*) "precision"
00101 #define XML_RANDOM (const xmlChar*) "random"
00103 #define XML_RELAXATION (const xmlChar*) "relaxation"
00104 #define XML_REPRODUCTION (const xmlChar*) "reproduction"
00106 #define XML_RESULT (const xmlChar*) "result"
00108 #define XML_SIMULATOR (const xmlChar*)"simulator
00109 #define XML_SEED (const xmlChar*) "seed"
```

```
00111 #define XML_STEP (const xmlChar*)"step"
00112 #define XML_SWEEP (const xmlChar*)"sweep"
00113 #define XML_TEMPLATE1 (const xmlChar*)"template1"
00114 #define XML_TEMPLATE2 (const xmlChar*)"template2"
00116 #define XML_TEMPLATE3 (const xmlChar*)"template3"
00118 #define XML_TEMPLATE4 (const xmlChar*)"template4"
00120 #define XML_TEMPLATE5 (const xmlChar*)"template5"
00122 #define XML_TEMPLATE6 (const xmlChar*)"template6"
00124 #define XML_TEMPLATE7 (const xmlChar*)"template6"
00126 #define XML_TEMPLATE8 (const xmlChar*)"template7"
00126 #define XML_TEMPLATE8 (const xmlChar*)"template8"
00128 #define XML_TOLERANCE (const xmlChar*)"tolerance"
00130 #define XML_VARIABLE (const xmlChar*)"variable"
00132 #define XML_VARIABLES (const xmlChar*)"variables"
00133 #define XML_WEIGHT (const xmlChar*)"weight"
00135
00136 #endif
```

5.3 interface.h File Reference

Header file of the interface.

This graph shows which files directly or indirectly include this file:



Data Structures

struct Experiment

Struct to define experiment data.

struct Variable

Struct to define variable data.

• struct Options

Struct to define the options dialog.

struct Running

Struct to define the running dialog.

struct Window

Struct to define the main window.

Macros

• #define MAX_LENGTH (DEFAULT_PRECISION + 8)

Max length of texts allowed in GtkSpinButtons.

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Functions

void input save (char *filename)

Function to save the input file.

void options new ()

Function to open the options dialog.

• void running_new ()

Function to open the running dialog.

• int window get algorithm ()

Function to get the stochastic algorithm number.

int window_get_gradient ()

Function to get the gradient base method number.

void window_save_gradient ()

Function to save the gradient based method data in the input file.

• int window_save ()

Function to save the input file.

• void window_run ()

Function to run a calibration.

void window_help ()

Function to show a help dialog.

void window_update_gradient ()

Function to update gradient based method widgets view in the main window.

• void window update ()

Function to update the main window view.

void window set algorithm ()

Function to avoid memory errors changing the algorithm.

void window set experiment ()

Function to set the experiment data in the main window.

void window_remove_experiment ()

Function to remove an experiment in the main window.

void window_add_experiment ()

Function to add an experiment in the main window.

void window_name_experiment ()

Function to set the experiment name in the main window.

void window_weight_experiment ()

Function to update the experiment weight in the main window.

• void window_inputs_experiment ()

Function to update the experiment input templates number in the main window.

void window_template_experiment (void *data)

Function to update the experiment i-th input template in the main window.

void window_set_variable ()

Function to set the variable data in the main window.

• void window_remove_variable ()

Function to remove a variable in the main window.

void window add variable ()

Function to add a variable in the main window.

void window_label_variable ()

Function to set the variable label in the main window.

· void window precision variable ()

Function to update the variable precision in the main window.

• void window_rangemin_variable ()

Function to update the variable rangemin in the main window.

void window_rangemax_variable ()

Function to update the variable rangemax in the main window.

void window rangeminabs variable ()

Function to update the variable rangeminabs in the main window.

void window_rangemaxabs_variable ()

Function to update the variable rangemaxabs in the main window.

• void window update variable ()

Function to update the variable data in the main window.

int window_read (char *filename)

Function to read the input data of a file.

• void window_open ()

Function to open the input data.

· void window new ()

Function to open the main window.

• int cores_number ()

Function to obtain the cores number.

5.3.1 Detailed Description

Header file of the interface.

Authors

Javier Burguete.

Copyright

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Definition in file interface.h.

5.3.2 Function Documentation

```
5.3.2.1 int cores_number ( )
```

Function to obtain the cores number.

Returns

Cores number.

Definition at line 4707 of file mpcotool.c.

```
04708 {
04709 #ifdef G_OS_WIN32
04710    SYSTEM_INFO sysinfo;
04711    GetSystemInfo (&sysinfo);
04712    return sysinfo.dwNumberOfProcessors;
04713 #else
04714    return (int) sysconf (_SC_NPROCESSORS_ONLN);
04715 #endif
04716 }
```

5.3.2.2 void input_save (char * filename)

Function to save the input file.

Parameters

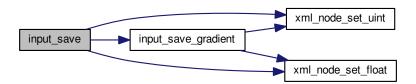
filename Input file name.

Definition at line 2670 of file mpcotool.c.

```
02671 {
02672
         unsigned int i, j;
02673
         char *buffer;
02674
         xmlDoc *doc;
02675
         xmlNode *node, *child;
02676
         GFile *file, *file2;
02677
         // Getting the input file directory
02678
02679
         input->name = g_path_get_basename (filename);
          input->directory = g_path_get_dirname (filename);
02680
         file = g_file_new_for_path (input->directory);
02682
02683
          // Opening the input file
02684
         doc = xmlNewDoc ((const xmlChar *) "1.0");
02685
02686
         // Setting root XML node
02687
         node = xmlNewDocNode (doc, 0, XML_CALIBRATE, 0);
02688
         xmlDocSetRootElement (doc, node);
02689
02690
         // Adding properties to the root XML node
         if (xmlStrcmp ((const xmlChar *) input->result, result_name))
   xmlSetProp (node, XML_RESULT, (xmlChar *) input->result);
02691
02692
02693
          if (xmlStrcmp ((const xmlChar *) input->variables,
       variables_name))
02694
           xmlSetProp (node, XML_VARIABLES, (xmlChar *) input->
      variables);
02695 file2 = g_file_new_for_path (input->simulator);
02696
         buffer = g_file_get_relative_path (file, file2);
02697
         g_object_unref (file2);
          xmlSetProp (node, XML_SIMULATOR, (xmlChar *) buffer);
02699
         g_free (buffer);
02700
          if (input->evaluator)
02701
           {
02702
              file2 = g_file_new_for_path (input->evaluator);
02703
              buffer = g_file_get_relative_path (file, file2);
02704
               g_object_unref (file2);
02705
               if (xmlStrlen ((xmlChar *) buffer))
02706
                 xmlSetProp (node, XML_EVALUATOR, (xmlChar *) buffer);
               g_free (buffer);
02707
02708
02709
         if (input->seed != DEFAULT_RANDOM_SEED)
02710
            xml_node_set_uint (node, XML_SEED, input->seed);
02711
02712
         // Setting the algorithm
02713
         buffer = (char *) g_malloc (64);
         switch (input->algorithm)
02714
02715
02716
            case ALGORITHM_MONTE_CARLO:
02717
               xmlSetProp (node, XML_ALGORITHM, XML_MONTE_CARLO);
02718
               snprintf (buffer, 64, "%u", input->nsimulations);
               xmlSetProp (node, XML_NSIMULATIONS, (xmlChar *) buffer);
02719
              snprintf (buffer, 64, "%u", input->niterations);
xmlSetProp (node, XML_NITERATIONS, (xmlChar *) buffer);
02720
02721
              snprintf (buffer, 64, "%.31g", input->tolerance);
xmlSetProp (node, XML_TOLERANCE, (xmlChar *) buffer);
02722
02723
02724
               snprintf (buffer, 64, "%u", input->nbest);
               xmlSetProp (node, XML_NBEST, (xmlChar *) buffer);
02725
02726
              input_save_gradient (node);
02727
              break:
            case ALGORITHM_SWEEP:
02728
              xmlSetProp (node, XML_ALGORITHM, XML_SWEEP);
02729
02730
               snprintf (buffer, 64, "%u", input->niterations);
02731
               xmlSetProp (node, XML_NITERATIONS, (xmlChar *) buffer);
              xmlsetriop (node, XML_NTERATION) (xmlchal *) buffer
snprintf (buffer, 64, "%.31g", input->tolerance);
xmlsetProp (node, XML_TOLERANCE, (xmlChar *) buffer);
snprintf (buffer, 64, "%u", input->nbest);
xmlSetProp (node, XML_NBEST, (xmlChar *) buffer);
02732
02733
02734
02735
02736
               input_save_gradient (node);
02737
02738
            default:
              xmlSetProp (node, XML_ALGORITHM, XML_GENETIC);
snprintf (buffer, 64, "%u", input->nsimulations);
xmlSetProp (node, XML_NPOPULATION, (xmlChar *) buffer);
02739
02740
02741
02742
               snprintf (buffer, 64, "%u", input->niterations);
02743
               xmlSetProp (node, XML_NGENERATIONS, (xmlChar *) buffer);
02744
               snprintf (buffer, 64, "%.31g", input->mutation_ratio);
              xmlSetProp (node, XML_MUTATION, (xmlChar *) buffer);
snprintf (buffer, 64, "%.31g", input->reproduction_ratio);
xmlSetProp (node, XML_REPRODUCTION, (xmlChar *) buffer);
02745
02746
              snprintf (buffer, 64, "%.31g", input->adaptation_ratio);
```

```
xmlSetProp (node, XML_ADAPTATION, (xmlChar *) buffer);
02750
            break;
02751
02752
        g_free (buffer);
02753
02754
        // Setting the experimental data
02755
        for (i = 0; i < input->nexperiments; ++i)
02756
02757
            child = xmlNewChild (node, 0, XML_EXPERIMENT, 0);
            xmlSetProp (child, XML_NAME, (xmlChar *) input->experiment[i]);
if (input->weight[i] != 1.)
02758
02759
              xml_node_set_float (child, XML_WEIGHT, input->
02760
      weight[i]);
02761
            for (j = 0; j < input->ninputs; ++j)
02762
              xmlSetProp (child, template[j], (xmlChar *) input->template[j][i]);
02763
02764
02765
        // Setting the variables data
        for (i = 0; i < input->nvariables; ++i)
02767
        {
            child = xmlNewChild (node, 0, XML_VARIABLE, 0);
xmlSetProp (child, XML_NAME, (xmlChar *) input->label[i]);
02768
02769
            xml_node_set_float (child, XML_MINIMUM, input->
02770
      rangemin[i]);
02771
         if (input->rangeminabs[i] != -G_MAXDOUBLE)
              xml_node_set_float (child, XML_ABSOLUTE_MINIMUM,
02772
      input->rangeminabs[i]);
02773
            xml_node_set_float (child, XML_MAXIMUM, input->
      rangemax[i]);
          if (input->rangemaxabs[i] != G_MAXDOUBLE)
02774
02775
             xml_node_set_float (child, XML_ABSOLUTE_MAXIMUM,
      input->rangemaxabs[i]);
02776
         if (input->precision[i] != DEFAULT_PRECISION)
02777
              xml_node_set_uint (child, XML_PRECISION,
      input->precision[i]);
02778
           if (input->algorithm == ALGORITHM_SWEEP)
02779
              xml_node_set_uint (child, XML_NSWEEPS, input->
      nsweeps[i]);
       else if (input->algorithm == ALGORITHM_GENETIC)
02780
02781
              xml_node_set_uint (child, XML_NBITS, input->
      nbits[i]);
02782
02783
02784
        // Saving the XML file
02785
       xmlSaveFormatFile (filename, doc, 1);
02786
02787
        // Freeing memory
02788
        xmlFreeDoc (doc);
02789 }
```

Here is the call graph for this function:



5.3.2.3 int window get_algorithm ()

Function to get the stochastic algorithm number.

Returns

Stochastic algorithm number.

Definition at line 2887 of file mpcotool.c.

5.3.2.4 int window_get_gradient ()

Function to get the gradient base method number.

Returns

Gradient base method number.

Definition at line 2903 of file mpcotool.c.

5.3.2.5 int window_read (char * filename)

Function to read the input data of a file.

Parameters

```
filename File name.
```

Returns

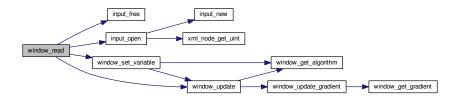
1 on succes, 0 on error.

Definition at line 3908 of file mpcotool.c.

```
03909 {
03910
       unsigned int i;
03911
        char *buffer;
03912 #if DEBUG
03913
       fprintf (stderr, "window_read: start\n");
03914 #endif
03915
03916
       // Reading new input file
03917
       input_free ();
03918
       if (!input_open (filename))
03919
          return 0;
03920
       // Setting GTK+ widgets data
03921
       gtk_entry_set_text (window->entry_result, input->result);
03922
03923
       gtk_entry_set_text (window->entry_variables, input->
     variables);
     buffer = g_build_filename (input->directory, input->
simulator, NULL);
03924
03925 gtk_file_chooser_set_filename (GTK_FILE_CHOOSER
03926
                                       (window->button simulator), buffer);
03927
       g_free (buffer);
03928
       gtk_toggle_button_set_active (GTK_TOGGLE_BUTTON (window->check_evaluator),
03929
                                      (size_t) input->evaluator);
03930
       if (input->evaluator)
03931
           buffer = g_build_filename (input->directory, input->
03932
     evaluator, NULL);
03933
            gtk_file_chooser_set_filename (GTK_FILE_CHOOSER
```

```
03934
                                            (window->button_evaluator), buffer);
03935
            g_free (buffer);
03936
03937
        {\tt gtk\_toggle\_button\_set\_active}
03938
          (GTK_TOGGLE_BUTTON (window->button_algorithm[input->
      algorithml), TRUE);
03939
       switch (input->algorithm)
03940
03941
          case ALGORITHM_MONTE_CARLO:
03942
            gtk_spin_button_set_value (window->spin_simulations,
03943
                                        (gdouble) input->nsimulations);
          case ALGORITHM SWEEP:
03944
03945
           gtk_spin_button_set_value (window->spin_iterations,
03946
                                        (gdouble) input->niterations);
03947
            gtk_spin_button_set_value (window->spin_bests, (gdouble)
      input->nbest);
03948
            gtk_spin_button_set_value (window->spin_tolerance,
      input->tolerance);
            gtk_toggle_button_set_active (GTK_TOGGLE_BUTTON (window->
      check_gradient),
03950
                                           input->nsteps);
03951
            if (input->nsteps)
03952
              {
03953
                {\tt gtk\_toggle\_button\_set\_active}
03954
                  (GTK_TOGGLE_BUTTON (window->button_gradient
                                       [input->gradient_method]), TRUE);
03955
                gtk_spin_button_set_value (window->spin_steps,
03956
03957
                                            (gdouble) input->nsteps);
03958
                gtk_spin_button_set_value (window->spin_relaxation,
03959
                                            (gdouble) input->relaxation);
03960
                switch (input->gradient_method)
03961
                  {
03962
                  case GRADIENT_METHOD_RANDOM:
03963
                    gtk_spin_button_set_value (window->spin_estimates,
03964
                                                (gdouble) input->nestimates);
03965
03966
              }
03967
            break;
03968
03969
            gtk_spin_button_set_value (window->spin_population,
03970
                                        (gdouble) input->nsimulations);
            gtk_spin_button_set_value (window->spin_generations,
03971
03972
                                        (gdouble) input->niterations);
03973
            gtk_spin_button_set_value (window->spin_mutation, input->
      mutation_ratio);
03974
            gtk_spin_button_set_value (window->spin_reproduction,
03975
                                        input->reproduction_ratio);
03976
            gtk_spin_button_set_value (window->spin_adaptation,
03977
                                        input->adaptation_ratio);
03978
03979
        g_signal_handler_block (window->combo_experiment, window->
      id_experiment);
03980
        g_signal_handler_block (window->button_experiment,
03981
                                 window->id_experiment_name);
        gtk_combo_box_text_remove_all (window->combo_experiment);
03982
        for (i = 0; i < input->nexperiments; ++i)
03983
03984
          gtk_combo_box_text_append_text (window->combo_experiment,
03985
                                           input->experiment[i]);
03986
        {\tt g\_signal\_handler\_unblock}
03987
          (window->button_experiment, window->
      id experiment name):
03988
        g_signal_handler_unblock (window->combo_experiment,
      window->id_experiment);
03989
      gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_experiment), 0);
03990
        g_signal_handler_block (window->combo_variable, window->
      id_variable);
03991
        g_signal_handler_block (window->entry_variable, window->
      id variable label);
        gtk_combo_box_text_remove_all (window->combo_variable);
03992
03993
        for
            (i = 0; i < input->nvariables; ++i)
          gtk_combo_box_text_append_text (window->combo_variable,
03994
      input->label[i]);
03995
        g_signal_handler_unblock (window->entry_variable, window->
      id variable label);
        g_signal_handler_unblock (window->combo_variable, window->
03996
     id_variable);
03997
       gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_variable), 0);
03998
        window_set_variable ();
03999
       window_update ();
04000
04001 #if DEBUG
04002
       fprintf (stderr, "window_read: end\n");
04003 #endif
04004
       return 1;
04005 }
```

Here is the call graph for this function:



```
5.3.2.6 int window_save ( )
```

Function to save the input file.

Returns

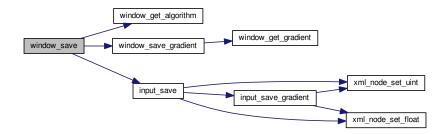
1 on OK, 0 on Cancel.

Definition at line 2951 of file mpcotool.c.

```
02952 {
02953
         char *buffer;
02954
        GtkFileChooserDialog *dlg;
02955
02956 #if DEBUG
02957
        fprintf (stderr, "window_save: start\n");
02958 #endif
02959
02960
         // Opening the saving dialog
02961
        dlg = (GtkFileChooserDialog *)
02962
           gtk_file_chooser_dialog_new (gettext ("Save file"),
02963
                                            window->window,
02964
                                            GTK_FILE_CHOOSER_ACTION_SAVE,
02965
                                            gettext ("_Cancel"),
02966
                                            GTK_RESPONSE_CANCEL,
02967
                                            gettext ("_OK"), GTK_RESPONSE_OK, NULL);
        gtk_file_chooser_set_do_overwrite_confirmation (GTK_FILE_CHOOSER (dlg), TRUE);
buffer = g_build_filename (input->directory, input->name, NULL);
02968
02969
02970
        gtk_file_chooser_set_filename (GTK_FILE_CHOOSER (dlg), buffer);
02971
        g_free (buffer);
02972
02973
         // If OK response then saving
02974
         if (gtk_dialog_run (GTK_DIALOG (dlg)) == GTK_RESPONSE_OK)
02975
02976
02977
             // Adding properties to the root XML node
02978
             input->simulator = gtk_file_chooser_get_filename
                (GTK_FILE_CHOOSER (window->button_simulator));
02979
02980
             if (gtk_toggle_button_get_active
  (GTK_TOGGLE_BUTTON (window->check_evaluator)))
02981
                input->evaluator = gtk_file_chooser_get_filename
  (GTK_FILE_CHOOSER (window->button_evaluator));
02982
02983
02984
02985
               input->evaluator = NULL;
02986
             input->result
02987
                = (char *) xmlStrdup ((const xmlChar *)
02988
                                        gtk_entry_get_text (window->entry_result));
02989
             input->variables
02990
                = (char *) xmlStrdup ((const xmlChar *)
02991
                                        gtk_entry_get_text (window->entry_variables));
02992
02993
             // Setting the algorithm
02994
             switch (window_get_algorithm ())
02995
02996
                case ALGORITHM_MONTE_CARLO:
02997
                  input->algorithm = ALGORITHM_MONTE_CARLO;
                  input->nsimulations
02998
02999
                  = gtk_spin_button_get_value_as_int (window->spin_simulations);
input->niterations
03000
03001
                    = gtk_spin_button_get_value_as_int (window->spin_iterations);
03002
                  input->tolerance = gtk_spin_button_get_value (window->
```

```
spin_tolerance);
03003
                input->nbest = gtk_spin_button_get_value_as_int (window->
      spin_bests);
03004
                window_save_gradient ();
03005
                break;
              case ALGORITHM_SWEEP:
03006
               input->algorithm = ALGORITHM_SWEEP;
03008
                input->niterations
03009
                  = gtk_spin_button_get_value_as_int (window->spin_iterations);
03010
                input->tolerance = gtk_spin_button_get_value (window->
      spin_tolerance);
03011
                input->nbest = gtk_spin_button_get_value_as_int (window->
     spin bests);
03012
                window_save_gradient ();
03013
                break;
03014
              default:
                input->algorithm = ALGORITHM GENETIC:
03015
               input->nsimulations
03016
03017
                  = gtk_spin_button_get_value_as_int (window->spin_population);
03018
                input->niterations
03019
                   -
= gtk_spin_button_get_value_as_int (window->spin_generations);
03020
03021
                  = gtk_spin_button_get_value (window->spin_mutation);
03022
                input->reproduction ratio
03023
                  = gtk_spin_button_get_value (window->spin_reproduction);
03024
                input->adaptation_ratio
03025
                   = gtk_spin_button_get_value (window->spin_adaptation);
03026
03027
              }
03028
03029
            // Saving the XML file
03030
            buffer = gtk_file_chooser_get_filename (GTK_FILE_CHOOSER (dlg));
03031
            input_save (buffer);
03032
            // Closing and freeing memory
g_free (buffer);
03033
03034
            gtk_widget_destroy (GTK_WIDGET (dlg));
03035
03036 #if DEBUG
03037
            fprintf (stderr, "window_save: end\n");
03038 #endif
03039
            return 1;
          }
03040
03041
03042
       // Closing and freeing memory
03043
        gtk_widget_destroy (GTK_WIDGET (dlg));
03044 #if DEBUG
03045
       fprintf (stderr, "window_save: end\n");
03046 #endif
03047
        return 0:
03048 }
```

Here is the call graph for this function:



5.3.2.7 void window_template_experiment (void * data)

Function to update the experiment i-th input template in the main window.

Parameters

data Callback data (i-th input template).

Definition at line 3544 of file mpcotool.c.

```
03545 {
03546
       unsigned int i, j;
03547
        char *buffer;
        GFile *file1, *file2;
03549 #if DEBUG
03550
       fprintf (stderr, "window_template_experiment: start\n");
03551 #endif
0.3552 i = (size t) data:
03553
        j = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_experiment));
03554
        filel
03555
          = gtk_file_chooser_get_file (GTK_FILE_CHOOSER (window->button_template[i]));
03556
       file2 = g_file_new_for_path (input->directory);
03557
        buffer = g_file_get_relative_path (file2, file1);
       input->template[i][j] = (char *) xmlStrdup ((xmlChar *) buffer);
03558
03559
        g_free (buffer);
03560
       g_object_unref (file2);
03561
        g_object_unref (file1);
03562 #if DEBUG
03563
       fprintf (stderr, "window_template_experiment: end\n");
03564 #endif
03565 }
```

5.4 interface.h

```
00002 MPCOTool: a software to make calibrations of empirical parameters.
00003
00004 AUTHORS: Javier Burguete and Borja Latorre.
00005
00006 Copyright 2012-2015, AUTHORS.
00007
00008 Redistribution and use in source and binary forms, with or without modification,
00009 are permitted provided that the following conditions are met:
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          1. Redistributions of source code must retain the above copyright notice,
00012
              this list of conditions and the following disclaimer.
00013
00014
          2. Redistributions in binary form must reproduce the above copyright notice,
00015
              this list of conditions and the following disclaimer in the
00016
              documentation and/or other materials provided with the distribution.
00017
00018 THIS SOFTWARE IS PROVIDED BY AUTHORS "AS IS" AND ANY EXPRESS OR IMPLIED
00019 WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF
00020 MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT
00021 SHALL AUTHORS OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL,
00022 SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO,
00023 PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR
00024 BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN 00025 CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING
00026 IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY
00027 OF SUCH DAMAGE.
00028 */
00029
00036 #ifndef INTERFACE__H
00037 #define INTERFACE H 1
00038
00039 #define MAX_LENGTH (DEFAULT_PRECISION + 8)
00040
00046 typedef struct
00047 {
       char *template[MAX_NINPUTS];
00048
00049
        char *name;
00050
        double weight;
00052 } Experiment;
00053
00058 typedef struct
00059 {
00060
       char *label;
00061
        double rangemin;
00062
        double rangemax;
00063
        double rangeminabs;
00064
        double rangemaxabs;
00065
       unsigned int precision;
00066
       unsigned int nsweeps:
       unsigned int nbits;
00068 } Variable;
```

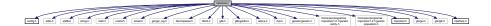
```
00069
00074 typedef struct
00075 {
00076
        GtkDialog *dialog;
00077
       GtkGrid *grid;
GtkLabel *label_seed;
00078
00080
        GtkSpinButton *spin_seed;
00082
        GtkLabel *label_threads;
00083
        GtkSpinButton *spin_threads;
00084
        GtkLabel *label_gradient;
00085
        GtkSpinButton *spin_gradient;
00086 } Options;
00087
00092 typedef struct
00093 {
00094
        GtkDialog *dialog;
00095
        GtkLabel *label:
00096 } Running;
00097
00102 typedef struct
00103 {
00104
        GtkWindow *window;
00105
        GtkGrid *grid;
00106
        GtkToolbar *bar buttons;
00107
        GtkToolButton *button_open;
00108
        GtkToolButton *button_save;
00109
        GtkToolButton *button_run;
00110
        GtkToolButton *button_options;
00111
        GtkToolButton *button_help;
00112
        GtkToolButton *button about:
00113
        GtkToolButton *button exit:
00114
        GtkGrid *grid_files;
00115
        GtkLabel *label_simulator;
00116
        GtkFileChooserButton *button_simulator;
00118
        GtkCheckButton *check_evaluator;
00119
        GtkFileChooserButton *button_evaluator;
00121
        GtkLabel *label_result;
00122
        GtkEntry *entry_result;
00123
        GtkLabel *label_variables;
00124
        GtkEntry *entry_variables;
00125
        GtkFrame *frame_algorithm;
00126
        GtkGrid *grid_algorithm;
        GtkRadioButton *button_algorithm[NALGORITHMS];
00127
00129
        GtkLabel *label_simulations;
00130
        GtkSpinButton *spin_simulations;
00132
        GtkLabel *label_iterations;
00133
        GtkSpinButton *spin_iterations;
00135
        GtkLabel *label tolerance;
00136
        GtkSpinButton *spin_tolerance;
        GtkLabel *label_bests;
00137
00138
        GtkSpinButton *spin_bests;
00139
        GtkLabel *label_population;
00140
        GtkSpinButton *spin_population;
00142
        GtkLabel *label_generations;
00143
        GtkSpinButton *spin_generations;
GtkLabel *label_mutation;
00145
00146
        GtkSpinButton *spin_mutation;
00147
        GtkLabel *label_reproduction;
00148
        GtkSpinButton *spin_reproduction;
00150
        GtkLabel *label_adaptation;
00151
        GtkSpinButton *spin_adaptation;
00153
        GtkCheckButton *check_gradient;
00155
        GtkGrid *grid_gradient;
00157
        GtkRadioButton *button_gradient[NGRADIENTS];
00159
        GtkLabel *label_steps;
00160
        GtkSpinButton *spin_steps;
00161
        GtkLabel *label estimates;
00162
        GtkSpinButton *spin_estimates;
        GtkLabel *label_relaxation;
00164
00166
        GtkSpinButton *spin_relaxation;
00168
        GtkFrame *frame_variable;
00169
        GtkGrid *grid_variable;
00170
        GtkComboBoxText *combo_variable;
00172
        GtkButton *button_add_variable;
00173
        GtkButton *button_remove_variable;
00174
        GtkLabel *label_variable;
00175
        GtkEntry *entry_variable;
00176
        GtkLabel *label_min;
00177
        GtkSpinButton *spin_min;
00178
        GtkScrolledWindow *scrolled min:
00179
        GtkLabel *label max;
00180
        GtkSpinButton *spin_max;
00181
        GtkScrolledWindow *scrolled_max;
00182
        GtkCheckButton *check_minabs;
00183
        GtkSpinButton *spin_minabs;
00184
        GtkScrolledWindow *scrolled minabs;
00185
        GtkCheckButton *check_maxabs;
```

```
GtkSpinButton *spin_maxabs;
00187
        GtkScrolledWindow *scrolled_maxabs;
00188
        GtkLabel *label_precision;
00189
        GtkSpinButton *spin_precision;
00190
        GtkLabel *label sweeps;
00191
        GtkSpinButton *spin sweeps:
00192
        GtkLabel *label_bits;
00193
        GtkSpinButton *spin_bits;
00194
        GtkFrame *frame_experiment;
00195
        GtkGrid *grid_experiment;
00196
        GtkComboBoxText *combo_experiment;
00197
        GtkButton *button_add_experiment;
00198
        GtkButton *button_remove_experiment;
00199
        GtkLabel *label_experiment;
00200
        GtkFileChooserButton *button_experiment;
00202
        GtkLabel *label_weight;
00203
        GtkSpinButton *spin_weight;
00204
        GtkCheckButton *check_template[MAX_NINPUTS];
00206
        GtkFileChooserButton *button_template[MAX_NINPUTS];
00208
        GdkPixbuf *logo;
00209
        Experiment *experiment;
00210
        Variable *variable;
       char *application_directory;
00211
00212
       gulong id_experiment;
qulong id_experiment_name;
00213
00214
       gulong id_variable;
00215
        gulong id_variable_label;
00216
        gulong id_template[MAX_NINPUTS];
00218
       gulong id_input[MAX_NINPUTS];
00220
       unsigned int nexperiments;
       unsigned int nvariables;
00221
00222 } Window;
00223
00224 // Public functions
00225 void input_save (char *filename);
00226 void options_new ();
00227 void running_new ();
00228 int window_get_algorithm ();
00229 int window_get_gradient ();
00230 void window_save_gradient ();
00231 int window_save ();
00232 void window_run ();
00233 void window_help ();
00234 void window_update_gradient ();
00235 void window_update ();
00236 void window_set_algorithm ();
00237 void window_set_experiment ();
00238 void window_remove_experiment ();
00239 void window_add_experiment ();
00240 void window_name_experiment ();
00241 void window_weight_experiment ();
00242 void window_inputs_experiment ();
00243 void window_template_experiment (void *data);
00244 void window_set_variable ();
00245 void window_remove_variable ();
00246 void window_add_variable ();
00247 void window_label_variable ();
00248 void window_precision_variable ();
00249 void window_rangemin_variable ();
00250 void window_rangemax_variable ();
00251 void window_rangeminabs_variable ();
00252 void window_rangemaxabs_variable ();
00253 void window_update_variable ();
00254 int window_read (char *filename);
00255 void window_open ();
00256 void window_new ();
00257 int cores_number ();
00258
00259 #endif
```

5.5 mpcotool.c File Reference

Source file of the mpcotool.

```
#include "config.h"
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <math.h>
#include <unistd.h>
#include <locale.h>
#include <gsl/gsl_rng.h>
#include <libxml/parser.h>
#include <libintl.h>
#include <glib.h>
#include <glib/gstdio.h>
#include <alloca.h>
#include <mpi.h>
#include "genetic/genetic.h"
#include "mpcotool.h"
#include <gio/gio.h>
#include <gtk/gtk.h>
#include "interface.h"
Include dependency graph for mpcotool.c:
```



Macros

- #define GNU SOURCE
- #define DEBUG 0

Macro to debug.

• #define ERROR_TYPE GTK_MESSAGE_ERROR

Macro to define the error message type.

• #define INFO_TYPE GTK_MESSAGE_INFO

Macro to define the information message type.

#define INPUT_FILE "test-ga.xml"

Macro to define the initial input file.

#define RM "rm"

Macro to define the shell remove command.

Functions

void show message (char *title, char *msg, int type)

Function to show a dialog with a message.

void show_error (char *msg)

Function to show a dialog with an error message.

• int xml_node_get_int (xmlNode *node, const xmlChar *prop, int *error_code)

Function to get an integer number of a XML node property.

• unsigned int xml_node_get_uint (xmlNode *node, const xmlChar *prop, int *error_code)

Function to get an unsigned integer number of a XML node property.

• double xml_node_get_float (xmlNode *node, const xmlChar *prop, int *error_code)

Function to get a floating point number of a XML node property.

void xml_node_set_int (xmlNode *node, const xmlChar *prop, int value)

Function to set an integer number in a XML node property.

void xml_node_set_uint (xmlNode *node, const xmlChar *prop, unsigned int value)

Function to set an unsigned integer number in a XML node property.

• void xml node set float (xmlNode *node, const xmlChar *prop, double value)

Function to set a floating point number in a XML node property.

• void input new ()

Function to create a new Input struct.

· void input free ()

Function to free the memory of the input file data.

• int input_open (char *filename)

Function to open the input file.

void calibrate_input (unsigned int simulation, char *input, GMappedFile *template)

Function to write the simulation input file.

• double calibrate_parse (unsigned int simulation, unsigned int experiment)

Function to parse input files, simulating and calculating the \ objective function.

• void calibrate print ()

Function to print the results.

· void calibrate_save_variables (unsigned int simulation, double error)

Function to save in a file the variables and the error.

void calibrate best (unsigned int simulation, double value)

Function to save the best simulations.

· void calibrate_sequential ()

Function to calibrate sequentially.

void * calibrate_thread (ParallelData *data)

Function to calibrate on a thread.

• void calibrate_merge (unsigned int nsaveds, unsigned int *simulation_best, double *error_best)

Function to merge the 2 calibration results.

void calibrate_synchronise ()

Function to synchronise the calibration results of MPI tasks.

void calibrate sweep ()

Function to calibrate with the sweep algorithm.

void calibrate_MonteCarlo ()

Function to calibrate with the Monte-Carlo algorithm.

void calibrate_best_gradient (unsigned int simulation, double value)

Function to save the best simulation in a gradient based method.

void calibrate_gradient_sequential (unsigned int simulation)

Function to estimate the gradient sequentially.

void * calibrate_gradient_thread (ParallelData *data)

Function to estimate the gradient on a thread.

double calibrate_estimate_gradient_random (unsigned int variable, unsigned int estimate)

Function to estimate a component of the gradient vector.

• double calibrate_estimate_gradient_coordinates (unsigned int variable, unsigned int estimate)

Function to estimate a component of the gradient vector.

void calibrate_step_gradient (unsigned int simulation)

Function to do a step of the gradient based method.

void calibrate_gradient ()

Function to calibrate with a gradient based method.

double calibrate_genetic_objective (Entity *entity)

Function to calculate the objective function of an entity.

void calibrate_genetic ()

Function to calibrate with the genetic algorithm.

 void calibrate_save_old () Function to save the best results on iterative methods. void calibrate merge old () Function to merge the best results with the previous step best results on iterative methods. • void calibrate_refine () Function to refine the search ranges of the variables in iterative algorithms. • void calibrate_step () Function to do a step of the iterative algorithm. • void calibrate iterate () Function to iterate the algorithm. • void calibrate free () Function to free the memory used by Calibrate struct. void calibrate_open ()

Function to open and perform a calibration.

void input_save_gradient (xmlNode *node)

Function to save the gradient based method data in a XML node.

void input_save (char *filename)

Function to save the input file.

void options_new ()

Function to open the options dialog.

void running_new ()

Function to open the running dialog.

int window_get_algorithm ()

Function to get the stochastic algorithm number.

int window_get_gradient ()

Function to get the gradient base method number.

void window_save_gradient ()

Function to save the gradient based method data in the input file.

• int window_save ()

Function to save the input file.

• void window_run ()

Function to run a calibration.

void window_help ()

Function to show a help dialog.

void window about ()

Function to show an about dialog.

void window update gradient ()

Function to update gradient based method widgets view in the main window.

void window_update ()

Function to update the main window view.

void window set algorithm ()

Function to avoid memory errors changing the algorithm.

void window_set_experiment ()

Function to set the experiment data in the main window.

void window_remove_experiment ()

Function to remove an experiment in the main window.

void window_add_experiment ()

Function to add an experiment in the main window.

void window name experiment ()

Function to set the experiment name in the main window.

void window_weight_experiment ()

Function to update the experiment weight in the main window.

• void window_inputs_experiment ()

Function to update the experiment input templates number in the main window.

void window_template_experiment (void *data)

Function to update the experiment i-th input template in the main window.

void window_set_variable ()

Function to set the variable data in the main window.

void window_remove_variable ()

Function to remove a variable in the main window.

• void window_add_variable ()

Function to add a variable in the main window.

void window_label_variable ()

Function to set the variable label in the main window.

void window precision variable ()

Function to update the variable precision in the main window.

void window_rangemin_variable ()

Function to update the variable rangemin in the main window.

void window_rangemax_variable ()

Function to update the variable rangemax in the main window.

void window_rangeminabs_variable ()

Function to update the variable rangeminabs in the main window.

void window rangemaxabs variable ()

Function to update the variable rangemaxabs in the main window.

• void window_update_variable ()

Function to update the variable data in the main window.

• int window_read (char *filename)

Function to read the input data of a file.

void window_open ()

Function to open the input data.

• void window new ()

Function to open the main window.

• int cores number ()

Function to obtain the cores number.

int main (int argn, char **argc)

Main function.

Variables

· int ntasks

Number of tasks.

unsigned int nthreads

Number of threads.

unsigned int nthreads_gradient

Number of threads for the gradient based method.

• GMutex mutex [1]

Mutex struct.

void(* calibrate_algorithm)()

Pointer to the function to perform a calibration algorithm step.

• double(* calibrate_estimate_gradient)(unsigned int variable, unsigned int estimate)

Pointer to the function to estimate the gradient.

• Input input [1]

Input struct to define the input file to mpcotool.

• Calibrate calibrate [1]

Calibration data.

const xmlChar * result_name = (xmlChar *) "result"

Name of the result file.

const xmlChar * variables_name = (xmlChar *) "variables"

Name of the variables file.

• const xmlChar * template [MAX_NINPUTS]

Array of xmlChar strings with template labels.

const char * format [NPRECISIONS]

Array of C-strings with variable formats.

const double precision [NPRECISIONS]

Array of variable precisions.

const char * logo []

Logo pixmap.

• Options options [1]

Options struct to define the options dialog.

Running running [1]

Running struct to define the running dialog.

• Window window [1]

Window struct to define the main interface window.

5.5.1 Detailed Description

Source file of the mpcotool.

Authors

Javier Burguete and Borja Latorre.

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Definition in file mpcotool.c.

5.5.2 Function Documentation

5.5.2.1 void calibrate_best (unsigned int simulation, double value)

Function to save the best simulations.

Parameters

simulation	Simulation number.
value	Objective function value.

Definition at line 1420 of file mpcotool.c.

```
01421 {
01422 unsigned int i, j;
01423 double e;
01424 #if DEBUG
01425 fprintf (stderr, "calibrate_best: start\n");
01426 fprintf (stderr, "calibrate_best: nsaveds=%u nbest=%u\n",
```

```
01427
                calibrate->nsaveds, calibrate->nbest);
01428 #endif
01429
      if (calibrate->nsaveds < calibrate->nbest
01430
           || value < calibrate->error_best[calibrate->nsaveds - 1])
01431
           if (calibrate->nsaveds < calibrate->nbest)
01432
             ++calibrate->nsaveds;
01433
01434
           calibrate->error_best[calibrate->nsaveds - 1] = value;
01435
          calibrate->simulation_best[calibrate->
for (i = calibrate->nsaveds; --i;)
01437
            {
01438
               if (calibrate->error_best[i] < calibrate->
     error_best[i - 1])
01439
                {
01440
                   j = calibrate->simulation_best[i];
                   e = calibrate->error_best[i];
01441
                  calibrate->simulation_best[i] = calibrate->
01442
     simulation_best[i - 1];
01443
                  calibrate->error_best[i] = calibrate->
     error_best[i - 1];
01444
                  calibrate->simulation_best[i - 1] = j;
                  calibrate->error_best[i - 1] = e;
01445
01446
                }
             else
01447
01448
                break;
01449
             }
01450
01451 #if DEBUG
01452 fprintf (stderr, "calibrate_best: end\n");
01453 #endif
01454 }
```

5.5.2.2 void calibrate best gradient (unsigned int simulation, double value)

Function to save the best simulation in a gradient based method.

Parameters

simulation	Simulation number.
value	Objective function value.

Definition at line 1733 of file mpcotool.c.

```
01734 {
01735 #if DEBUG
01736 fprintf (stderr, "calibrate_best_gradient: start\n");
01737 fprintf (stderr,
       fprintf (stderr,
01738
                 "calibrate_best_gradient: simulation=%u value=%.14le best=%.14le\n",
01739
                 simulation, value, calibrate->error_best[0]);
01740 #endif
01741 if (value < calibrate->error_best[0])
01742
        {
01743
           calibrate->error_best[0] = value;
01744
            calibrate->simulation_best[0] = simulation;
01745 #if DEBUG
       fprintf (stderr,
01746
01747
                     "calibrate best gradient: BEST simulation=%u value=%.14le\n",
01748
                     simulation, value);
01749 #endif
01750 }
01751 #if DEBUG
01752 fprintf (stderr, "calibrate_best_gradient: end\n");
01753 #endif
01754 }
```

5.5.2.3 double calibrate estimate gradient coordinates (unsigned int variable, unsigned int estimate)

Function to estimate a component of the gradient vector.

Parameters

variable	Variable number.
estimate	Estimate number.

Definition at line 1870 of file mpcotool.c.

```
01872 {
                                   double x;
 01874 #if DEBUG
 01875
                                  fprintf (stderr, "calibrate_estimate_gradient_coordinates: start\n");
 01876 #endif
                              x = calibrate->gradient[variable];
 01877
 01878
                                if (estimate >= (2 * variable) && estimate < (2 * variable + 2))</pre>
 01879
                                     {
 01880
                                                     if (estimate & 1)
 01881
                                                             x += calibrate->step[variable];
 01882
                                                     else
 01883
                                                           x -= calibrate->step[variable];
 01884
 01885 #if DEBUG
 01886 fprintf (stderr, "calibrate_estimate_gradient_coordinates: gradient%u=%lg\n", "calibrate_estimate_gradient_coordinates: gradient_gradient_coordinates: gradient_gradient_coordinates: gradient_gradient_coordinates: gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradient_gradi
                                variable, x);
fprintf (stderr, "calibrate_estimate_gradient_coordinates: end\n");
 01887
 01888
 01889 #endif
01890
                              return x;
01891 }
```

5.5.2.4 double calibrate estimate gradient random (unsigned int variable, unsigned int estimate)

Function to estimate a component of the gradient vector.

Parameters

variable	Variable number.
estimate	Estimate number.

Definition at line 1843 of file mpcotool.c.

```
01845 {
01846
       double x;
01847 #if DEBUG
01848
       fprintf (stderr, "calibrate_estimate_gradient_random: start\n");
01849 #endif
01850 x = calibrate->gradient[variable]
         + (1. - 2. * gsl_rng_uniform (calibrate->rng)) * calibrate->
01851
     step[variable];
01852 #if DEBUG
01853 fprintf (stderr, "calibrate_estimate_gradient_random: gradient%u=%lg\n",
       variable, x);
fprintf (stderr, "calibrate_estimate_gradient_random: end\n");
01854
01855
01856 #endif
01857 return x;
01858 }
```

5.5.2.5 double calibrate_genetic_objective (Entity * entity)

Function to calculate the objective function of an entity.

Parameters

entity entity data.

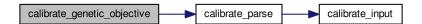
Returns

objective function value.

Definition at line 2036 of file mpcotool.c.

```
02037 {
02038
        unsigned int j;
02039
        double objective;
02040
        char buffer[64];
02041 #if DEBUG
02042
        fprintf (stderr, "calibrate_genetic_objective: start\n");
02043 #endif
02044
        for (j = 0; j < calibrate->nvariables; ++j)
02045
02046
            calibrate->value[entity->id * calibrate->nvariables + j]
02047
              = genetic_get_variable (entity, calibrate->genetic_variable + j);
02048
02049
        for (j = 0, objective = 0.; j < calibrate->nexperiments; ++j)
02050
         objective += calibrate_parse (entity->id, j);
02051
        g_mutex_lock (mutex);
        for (j = 0; j < calibrate->nvariables; ++j)
02052
02053
            snprintf (buffer, 64, "%s ", format[calibrate->precision[j]]);
fprintf (calibrate->file_variables, buffer,
02054
02055
02056
                      genetic_get_variable (entity, calibrate->
      genetic_variable + j));
02057
        fprintf (calibrate->file_variables, "%.14le\n", objective);
02058
02059
        g_mutex_unlock (mutex);
02060 #if DEBUG
        fprintf (stderr, "calibrate_genetic_objective: end\n");
02062 #endif
02063
        return objective;
02064 }
```

Here is the call graph for this function:



5.5.2.6 void calibrate_gradient_sequential (unsigned int simulation)

Function to estimate the gradient sequentially.

Parameters

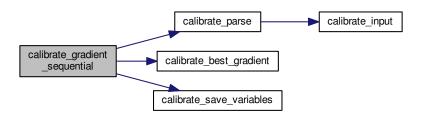
```
simulation | Simulation number.
```

Definition at line 1763 of file mpcotool.c.

```
01764 {
01765
         unsigned int i, j, k;
01766
         double e:
01767 #if DEBUG
       fprintf (stderr, "calibrate_gradient_sequential: start\n");
fprintf (stderr, "calibrate_gradient_sequential: nstart_gradient=%u "
01769
01770
                    "nend_gradient=%un",
01771
                    calibrate->nstart_gradient, calibrate->
       nend_gradient);
01772 #endif
01773
         for (i = calibrate->nstart_gradient; i < calibrate->nend_gradient; ++i)
01774
01775
              k = simulation + i;
              e = 0.;
01776
              for (j = 0; j < calibrate->nexperiments; ++j)
  e += calibrate_parse (k, j);
calibrate_best_gradient (k, e);
01777
01778
01779
01780
              calibrate_save_variables (k, e);
01781 #if DEBUG
01782
              fprintf (stderr, "calibrate_gradient_sequential: i=u = lg n", i, e);
01783 #endif
01784
01785 #if DEBUG
01786
        fprintf (stderr, "calibrate_gradient_sequential: end\n");
```

```
01787 #endif
01788 }
```

Here is the call graph for this function:



5.5.2.7 void * calibrate_gradient_thread (ParallelData * data)

Function to estimate the gradient on a thread.

Parameters

data	Function data.

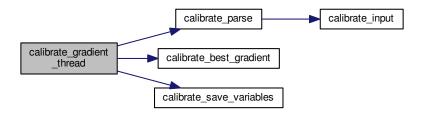
Returns

NULL

Definition at line 1798 of file mpcotool.c.

```
01800
        unsigned int i, j, thread;
01801
        double e;
01802 #if DEBUG
        fprintf (stderr, "calibrate_gradient_thread: start\n");
01803
01804 #endif
01805
        thread = data->thread;
01806 #if DEBUG
01807 fprintf (stderr, "calibrate_gradient_thread: thread=%u start=%u end=%un",
01808
                  thread,
01809
                  calibrate->thread_gradient[thread],
calibrate->thread_gradient[thread + 1]);
01810
01811 #endif
        for (i = calibrate->thread_gradient[thread];
01813
              i < calibrate->thread_gradient[thread + 1]; ++i)
01814
01815
            e = 0.;
            for (j = 0; j < calibrate->nexperiments; ++j)
e += calibrate_parse (i, j);
01816
01817
            g_mutex_lock (mutex);
01818
01819
             calibrate_best_gradient (i, e);
01820
            calibrate_save_variables (i, e);
01821
             g_mutex_unlock (mutex);
01822 #if DEBUG
             fprintf (stderr, "calibrate_gradient_thread: i=%u e=%lg\n", i, e);
01823
01824 #endif
01825
01826 #if DEBUG
01827
        fprintf (stderr, "calibrate_gradient_thread: end\n");
01828 #endif
01829
        g_thread_exit (NULL);
01830
        return NULL;
01831 }
```

Here is the call graph for this function:



5.5.2.8 void calibrate_input (unsigned int simulation, char * input, GMappedFile * template)

Function to write the simulation input file.

Parameters

simulation	Simulation number.
input	Input file name.
template	Template of the input file name.

Definition at line 1173 of file mpcotool.c.

```
01174 {
01175
        unsigned int i;
01176
        char buffer[32], value[32], *buffer2, *buffer3, *content;
01177
       FILE *file;
01178
        gsize length;
01179
       GRegex *regex:
01180
01181 #if DEBUG
01182
       fprintf (stderr, "calibrate_input: start\n");
01183 #endif
01184
01185
        // Checking the file
01186
       if (!template)
01187
         goto calibrate_input_end;
01188
01189
       // Opening template
       content = g_mapped_file_get_contents (template);
01190
        length = g_mapped_file_get_length (template);
01191
01192 #if DEBUG
01193
      fprintf (stderr, "calibrate_input: length=%lu\ncontent:\n%s", length,
01194
                 content);
01195 #endif
       file = g_fopen (input, "w");
01196
01197
01198
       // Parsing template
01199
       for (i = 0; i < calibrate->nvariables; ++i)
01200
01201 #if DEBUG
01202
            fprintf (stderr, "calibrate_input: variable=%u\n", i);
01203 #endif
01204
            snprintf (buffer, 32, "@variable%u@", i + 1);
01205
            regex = g_regex_new (buffer, 0, 0, NULL);
01206
            if(i == 0)
01207
01208
               buffer2 = g_regex_replace_literal (regex, content, length, 0,
01209
                                                    calibrate->label[i], 0, NULL);
01210 #if DEBUG
01211
                fprintf (stderr, "calibrate_input: buffer2\n%s", buffer2);
01212 #endif
01213
01214
            else
01215
01216
                length = strlen (buffer3);
01217
                buffer2 = g_regex_replace_literal (regex, buffer3, length, 0,
01218
                                                    calibrate->label[i], 0, NULL);
```

```
01219
                 g_free (buffer3);
01220
01221
             g_regex_unref (regex);
             length = strlen (buffer2);
snprintf (buffer, 32, "@value%u@", i + 1);
01222
01223
             regex = g_regex_new (buffer, 0, 0, NULL);
snprintf (value, 32, format[calibrate->precision[i]],
01224
01225
01226
                        calibrate->value[simulation * calibrate-
nvariables + i]);
01228 #if DEBUG
             fprintf (stderr, "calibrate_input: value=%s\n", value);
01229
01230 #endif
01231
             buffer3 = g_regex_replace_literal (regex, buffer2, length, 0, value,
01232
                                                    0, NULL);
01233
             g_free (buffer2);
01234
             g_regex_unref (regex);
         }
01235
01236
01237
        // Saving input file
01238
        fwrite (buffer3, strlen (buffer3), sizeof (char), file);
01239 g_free (buffer3);
01240 fclose (file);
01241
01242 calibrate_input_end:
01243 #if DEBUG
01244
        fprintf (stderr, "calibrate_input: end\n");
01245 #endif
01246
        return;
01247 }
```

5.5.2.9 void calibrate_merge (unsigned int *simulation_best, double *error_best)

Function to merge the 2 calibration results.

Parameters

nsaveds	Number of saved results.
simulation_best	Array of best simulation numbers.
error_best	Array of best objective function values.

Definition at line 1538 of file mpcotool.c.

```
01540 {
01541
        unsigned int i, j, k, s[calibrate->nbest];
        double e[calibrate->nbest];
01542
01543 #if DEBUG
01544
       fprintf (stderr, "calibrate_merge: start\n");
01545 #endif
      i = j = k = 0;
01546
01547
       do
01548
        {
01549
            if (i == calibrate->nsaveds)
01550
             {
01551
               s[k] = simulation_best[j];
01552
                e[k] = error_best[j];
01553
               ++j;
01554
               ++k;
01555
               if (j == nsaveds)
01556
                 break;
01558
            else if (j == nsaveds)
01559
01560
               s[k] = calibrate->simulation_best[i];
                e[k] = calibrate->error_best[i];
01561
01562
               ++i;
01563
               ++k;
01564
               if (i == calibrate->nsaveds)
01565
                 break;
01566
01567
            else if (calibrate->error_best[i] > error_best[j])
01568
             {
                s[k] = simulation_best[j];
01569
01570
                e[k] = error_best[j];
01571
                ++j;
                ++k;
01572
01573
01574
            else
01575
01576
                s[k] = calibrate->simulation_best[i];
```

```
e[k] = calibrate->error_best[i];
01578
01579
                ++k;
             }
01580
01581
       while (k < calibrate->nbest);
01582
       calibrate->nsaveds = k;
01583
       memcpy (calibrate->simulation_best, s, k * sizeof (unsigned int));
01584
01585
       memcpy (calibrate->error_best, e, k * sizeof (double));
01586 #if DEBUG
       fprintf (stderr, "calibrate_merge: end\n");
01587
01588 #endif
01589 }
```

5.5.2.10 double calibrate_parse (unsigned int simulation, unsigned int experiment)

Function to parse input files, simulating and calculating the \ objective function.

Parameters

simulation	Simulation number.
experiment	Experiment number.

Returns

Objective function value.

Definition at line 1260 of file mpcotool.c.

```
01261 {
01262
        unsigned int i:
01263
        double e:
       char buffer[512], input[MAX_NINPUTS][32], output[32], result[32], *buffer2,
01264
          *buffer3, *buffer4;
01265
01266
       FILE *file_result;
01267
01268 #if DEBUG
       fprintf (stderr, "calibrate_parse: start\n");
fprintf (stderr, "calibrate_parse: simulation=%u experiment=%u\n", simulation,
01269
01270
                 experiment);
01272 #endif
01273
01274
        // Opening input files
01275
        for (i = 0; i < calibrate->ninputs; ++i)
01276
01277
            snprintf (&input[i][0], 32, "input-%u-%u-%u", i, simulation, experiment);
01278 #if DEBUG
01279
            fprintf (stderr, "calibrate_parse: i=%u input=%sn", i, &input[i][0]);
01280 #endif
01281
            01282
01283
01284
        for (; i < MAX_NINPUTS; ++i)</pre>
01285
          strcpy (&input[i][0], "");
01286 #if DEBUG
       fprintf (stderr, "calibrate_parse: parsing end\n");
01287
01288 #endif
01289
        // Performing the simulation
01291
        snprintf (output, 32, "output-%u-%u", simulation, experiment);
01292
        buffer2 = g_path_get_dirname (calibrate->simulator);
        buffer3 = g_path_get_basename (calibrate->simulator);
01293
        buffer4 = g_build_filename (buffer2, buffer3, NULL);
01294
       snprintf (buffer, 512, "\"%s\" %s ",

buffer4, input[0], input[1], input[2], input[3], input[4], input[5],
01295
01296
01297
                  input[6], input[7], output);
01298
       g_free (buffer4);
01299
        g_free (buffer3);
01300
        g_free (buffer2);
01301 #if DEBUG
01302
        fprintf (stderr, "calibrate_parse: %s\n", buffer);
01303 #endif
01304
       system (buffer);
01305
01306
        // Checking the objective value function
01307
        if (calibrate->evaluator)
01308
01309
            snprintf (result, 32, "result-%u-%u", simulation, experiment);
```

```
buffer2 = g_path_get_dirname (calibrate->evaluator);
01311
            buffer3 = g_path_get_basename (calibrate->evaluator);
            buffer4 = g_build_filename (buffer2, buffer3, NULL); snprintf (buffer, 512, "\"%s\" %s %s %s",
01312
01313
01314
                      buffer4, output, calibrate->experiment[experiment], result);
01315
            g_free (buffer4);
01316
            g_free (buffer3);
01317
            g_free (buffer2);
01318 #if DEBUG
01319 fprintf (stderr, "calibrate_parse: n'', buffer); 01320 #endif
01321
           system (buffer);
            file_result = g_fopen (result, "r");
e = atof (fgets (buffer, 512, file_result));
01322
01323
01324
            fclose (file_result);
01325
01326
       else
01327
        {
           strcpy (result, "");
01328
           file_result = g_fopen (output, "r");
01330
            e = atof (fgets (buffer, 512, file_result));
01331
            fclose (file_result);
         }
01332
01333
01334
        // Removing files
01335 #if !DEBUG
        for (i = 0; i < calibrate->ninputs; ++i)
01336
01337
            if (calibrate->file[i][0])
01338
01339
              {
01340
                snprintf (buffer, 512, RM " %s", &input[i][0]);
01341
                system (buffer);
01342
01343
01344
       snprintf (buffer, 512, RM " %s %s", output, result);
01345
        system (buffer);
01346 #endif
01347
01348 #if DEBUG
01349
       fprintf (stderr, "calibrate_parse: end\n");
01350 #endif
01351
        // Returning the objective function
01352
01353
        return e * calibrate->weight[experiment];
01354 }
```

Here is the call graph for this function:



5.5.2.11 void calibrate_save_variables (unsigned int *simulation*, double *error*)

Function to save in a file the variables and the error.

Parameters

simulation	Simulation number.
error	Error value.

Definition at line 1392 of file mpcotool.c.

```
01393 {
01394 unsigned int i;
01395 char buffer[64];
01396 #if DEBUG
```

```
fprintf (stderr, "calibrate_save_variables: start\n");
01398 #endif
        for (i = 0; i < calibrate->nvariables; ++i)
01399
01400
             snprintf (buffer, 64, "%s ", format[calibrate->precision[i]]);
fprintf (calibrate->file_variables, buffer,
01401
01402
                       calibrate->value[simulation * calibrate->
01403
      nvariables + i]);
01404
        fprintf (calibrate->file_variables, "%.14le\n", error);
01405
01406 #if DEBUG
        fprintf (stderr, "calibrate_save_variables: end\n");
01407
01408 #endif
01409 }
```

5.5.2.12 void calibrate_step_gradient (unsigned int simulation)

Function to do a step of the gradient based method.

Parameters

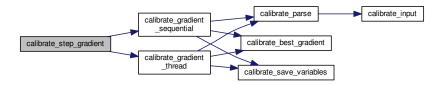
simulation | Simulation number.

Definition at line 1900 of file mpcotool.c.

```
01901 {
01902
        GThread *thread[nthreads_gradient];
01903
        ParallelData data[nthreads_gradient];
01904
        unsigned int i, j, k, b;
01905 #if DEBUG
        fprintf (stderr, "calibrate_step_gradient: start\n");
01907 #endif
01908
       for (i = 0; i < calibrate->nestimates; ++i)
01909
           k = (simulation + i) * calibrate > nvariables:
01910
            b = calibrate->simulation_best[0] * calibrate->
01911
      nvariables;
01912 #if DEBUG
01913
           fprintf (stderr, "calibrate_step_gradient: simulation=%u best=%u\n",
01914
                     simulation + i, calibrate->simulation_best[0]);
01915 #endif
01916
           for (j = 0; j < calibrate->nvariables; ++j, ++k, ++b)
01917
01918 #if DEBUG
01919
              fprintf (stderr,
01920
                         "calibrate_step_gradient: estimate=%u best%u=%.14le\n",
01921
                         i, j, calibrate->value[b]);
01922 #endif
01923
               calibrate->value[k]
01924
                   = calibrate->value[b] + calibrate_estimate_gradient (j
, i);
01925
                calibrate->value[k] = fmin (fmax (calibrate->
     value[k].
01926
                                                   calibrate->rangeminabs[j]),
01927
                                            calibrate->rangemaxabs[j]);
01928 #if DEBUG
01929
               fprintf (stderr,
01930
                         "calibrate_step_gradient: estimate=%u variable%u=%.14le\n",
01931
                         i, j, calibrate->value[k]);
01932 #endif
01933
01935
        if (nthreads_gradient == 1)
01936
         calibrate_gradient_sequential (simulation);
01937
        else
01938
         {
01939
            for (i = 0; i <= nthreads_gradient; ++i)</pre>
01940
01941
                calibrate->thread_gradient[i]
01942
                  = simulation + calibrate->nstart_gradient
                  + i * (calibrate->nend_gradient - calibrate->
01943
     nstart_gradient)
01944
                 / nthreads_gradient;
01945 #if DEBUG
01946
               fprintf (stderr,
01947
                         "calibrate_step_gradient: i=%u thread_gradient=%u\n",
01948
                         i, calibrate->thread_gradient[i]);
01949 #endif
01950
01951
            for (i = 0; i < nthreads_gradient; ++i)</pre>
01952
```

```
01953
                data[i].thread = i;
01954
                thread[i] = g_thread_new
01955
                   (NULL, (void (*)) calibrate_gradient_thread, &data[i]);
01956
            for (i = 0; i < nthreads_gradient; ++i)</pre>
01957
              g_thread_join (thread[i]);
01958
01959
01960 #if DEBUG
01961
       fprintf (stderr, "calibrate_step_gradient: end\n");
01962 #endif
01963 }
```

Here is the call graph for this function:



5.5.2.13 void * calibrate_thread (ParallelData * data)

Function to calibrate on a thread.

Parameters

data	Function data.

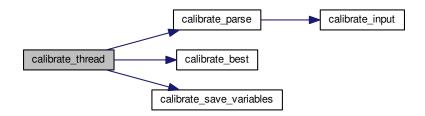
Returns

NULL

Definition at line 1494 of file mpcotool.c.

```
01495 {
01496
        unsigned int i, j, thread;
01497
        double e;
01498 #if DEBUG
01499
       fprintf (stderr, "calibrate_thread: start\n");
01500 #endif
01501
        thread = data->thread;
01502 #if DEBUG
        fprintf (stderr, "calibrate_thread: thread=%u start=%u end=%u\n", thread,
01503
01504
                 calibrate->thread[thread], calibrate->thread[thread + 1]);
01505 #endif
01506
       for (i = calibrate->thread[thread]; i < calibrate->thread[thread + 1]; ++i)
01507
            e = 0.;
01508
            for (j = 0; j < calibrate->nexperiments; ++j)
  e += calibrate_parse (i, j);
01509
01510
01511
            g_mutex_lock (mutex);
01512
            calibrate_best (i, e);
01513
            calibrate_save_variables (i, e);
01514
            g_mutex_unlock (mutex);
01515 #if DEBUG
            fprintf (stderr, "calibrate_thread: i=%u e=%lgn", i, e);
01516
01517 #endif
01518
01519 #if DEBUG
01520
       fprintf (stderr, "calibrate_thread: end\n");
01521 #endif
01522
       g_thread_exit (NULL);
01523
        return NULL;
01524 }
```

Here is the call graph for this function:



```
5.5.2.14 int cores_number ( )
```

Function to obtain the cores number.

Returns

Cores number.

Definition at line 4707 of file mpcotool.c.

```
04708 {
04709 #ifdef G_OS_WIN32
04710    SYSTEM_INFO sysinfo;
04711    GetSystemInfo (&sysinfo);
04712    return sysinfo.dwNumberOfProcessors;
04713 #else
04714    return (int) sysconf (_SC_NPROCESSORS_ONLN);
04715 #endif
04716 }
```

5.5.2.15 int input_open (char * filename)

Function to open the input file.

Parameters

```
filename Input data file name.
```

Returns

1 on success, 0 on error.

Definition at line 488 of file mpcotool.c.

```
00489 {
 00490
                                                             char buffer2[64];
                                                            char *buffert[MAX_NINPUTS] =
    { NULL, NU
 00491
 00492
                                                          xmlDoc *doc;
xmlNode *node, *child;
00493
 00494
 00495
                                                             xmlChar *buffer;
 00496
                                                            char *msg;
 00497
                                                             int error_code;
 00498
                                                          unsigned int i;
 00499
00500 #if DEBUG
00501 fprintf (stderr, "input_open: start\n");
00502 #endif
```

```
00503
00504
        // Resetting input data
00505
        buffer = NULL;
00506
       input_new ();
00507
00508
        // Parsing the input file
00509 #if DEBUG
00510
       fprintf (stderr, "input_open: parsing the input file %s\n", filename);
00511 #endif
       doc = xmlParseFile (filename);
00512
00513
        if (!doc)
00514
         {
00515
            msg = gettext ("Unable to parse the input file");
00516
            goto exit_on_error;
00517
00518
        // Getting the root node
00519
00520 #if DEBUG
00521
       fprintf (stderr, "input_open: getting the root node\n");
00522 #endif
00523
        node = xmlDocGetRootElement (doc);
00524
        if (xmlStrcmp (node->name, XML_CALIBRATE))
00525
           msg = gettext ("Bad root XML node");
00526
00527
            goto exit_on_error;
00528
00529
00530
        // Getting results file names
00531
        input->result = (char *) xmlGetProp (node, XML_RESULT);
00532
        if (!input->result)
00533
          input->result = (char *) xmlStrdup (result name);
00534
        input->variables = (char *) xmlGetProp (node, XML_VARIABLES);
00535
        if (!input->variables)
00536
          input->variables = (char *) xmlStrdup (variables_name);
00537
00538
        // Opening simulator program name
00539
        input->simulator = (char *) xmlGetProp (node, XML_SIMULATOR);
00540
        if (!input->simulator)
00541
         {
00542
            msg = gettext ("Bad simulator program");
00543
            goto exit_on_error;
          }
00544
00545
00546
        // Opening evaluator program name
00547
        input->evaluator = (char *) xmlGetProp (node, XML_EVALUATOR);
00548
00549
        // Obtaining pseudo-random numbers generator seed
        if (!xmlHasProp (node, XML_SEED))
input->seed = DEFAULT_RANDOM_SEED;
00550
00551
00552
        else
00553
         {
00554
            input->seed = xml_node_get_uint (node, XML_SEED, &error_code);
00555
            if (error_code)
00556
00557
                msg = gettext ("Bad pseudo-random numbers generator seed");
00558
                goto exit_on_error;
00559
00560
00561
00562
        // Opening algorithm
        buffer = xmlGetProp (node, XML_ALGORITHM);
if (!xmlStrcmp (buffer, XML_MONTE_CARLO))
00563
00564
00565
00566
            input->algorithm = ALGORITHM_MONTE_CARLO;
00567
00568
            // Obtaining simulations number
00569
            input->nsimulations
00570
              = xml_node_get_int (node, XML_NSIMULATIONS, &error_code);
00571
            if (error_code)
00572
             {
00573
               msg = gettext ("Bad simulations number");
00574
                goto exit_on_error;
              }
00575
00576
          }
00577
        else if (!xmlStrcmp (buffer, XML_SWEEP))
         input->algorithm = ALGORITHM_SWEEP;
00578
00579
        else if (!xmlStrcmp (buffer, XML_GENETIC))
00580
            input->algorithm = ALGORITHM_GENETIC;
00581
00582
00583
            // Obtaining population
00584
            if (xmlHasProp (node, XML_NPOPULATION))
00585
00586
                input->nsimulations
00587
                  = xml_node_get_uint (node, XML_NPOPULATION, &error_code);
00588
                if (error_code || input->nsimulations < 3)</pre>
00589
```

```
msg = gettext ("Invalid population number");
00591
                     goto exit_on_error;
00592
                   }
00593
00594
            else
00595
              {
                msg = gettext ("No population number");
00596
00597
                 goto exit_on_error;
00598
00599
00600
             // Obtaining generations
            if (xmlHasProp (node, XML_NGENERATIONS))
00601
00602
              {
00603
                 input->niterations
00604
                   = xml_node_get_uint (node, XML_NGENERATIONS, &error_code);
00605
                 if (error_code || !input->niterations)
00606
00607
                     msg = gettext ("Invalid generations number");
00608
                     goto exit_on_error;
00609
                   }
00610
00611
            else
00612
              {
                msg = gettext ("No generations number");
00613
00614
                goto exit_on_error;
00615
00616
00617
             // Obtaining mutation probability
00618
            if (xmlHasProp (node, XML_MUTATION))
00619
               {
00620
                 input->mutation_ratio
                 = xml_node_get_float (node, XML_MUTATION, &error_code);
if (error_code || input->mutation_ratio < 0.</pre>
00621
00622
00623
                     || input->mutation_ratio >= 1.)
00624
                     msg = gettext ("Invalid mutation probability");
00625
00626
                     goto exit_on_error;
00627
00628
00629
            else
00630
              {
                msg = gettext ("No mutation probability");
00631
00632
                goto exit_on_error;
00633
00634
00635
             // Obtaining reproduction probability
00636
             if (xmlHasProp (node, XML_REPRODUCTION))
00637
00638
                 input->reproduction ratio
                   = xml_node_get_float (node, XML_REPRODUCTION, &error_code);
00639
                 if (error_code || input->reproduction_ratio < 0.</pre>
00640
00641
                     || input->reproduction_ratio >= 1.0)
00642
00643
                     msg = gettext ("Invalid reproduction probability");
00644
                     goto exit_on_error;
                   }
00645
00646
              }
00647
            else
00648
00649
                 msg = gettext ("No reproduction probability");
00650
                goto exit_on_error;
00651
00652
00653
             // Obtaining adaptation probability
00654
            if (xmlHasProp (node, XML_ADAPTATION))
00655
00656
                 input->adaptation_ratio
                 = xml_node_get_float (node, XML_ADAPTATION, &error_code);
if (error_code || input->adaptation_ratio < 0.</pre>
00657
00658
                     || input->adaptation_ratio >= 1.)
00660
00661
                     msg = gettext ("Invalid adaptation probability");
00662
                     goto exit_on_error;
00663
00664
               }
00665
            else
00666
              {
00667
                 msg = gettext ("No adaptation probability");
00668
                 goto exit_on_error;
              }
00669
00670
00671
             // Checking survivals
00672
             i = input->mutation_ratio * input->nsimulations;
00673
            i += input->reproduction_ratio * input->
      nsimulations;
00674
           i += input->adaptation_ratio * input->
      nsimulations;
```

```
if (i > input->nsimulations - 2)
00676
00677
                msg = gettext
                  ("No enough survival entities to reproduce the population");
00678
00679
                goto exit_on_error;
00680
              }
00681
00682
        else
00683
        {
            msg = gettext ("Unknown algorithm");
00684
00685
            goto exit_on_error;
00686
00687
        xmlFree (buffer);
        buffer = NULL;
00688
00689
00690
        if (input->algorithm == ALGORITHM_MONTE_CARLO
00691
            || input->algorithm == ALGORITHM_SWEEP)
        {
00692
00693
00694
            // Obtaining iterations number
00695
            input->niterations
00696
              = xml_node_get_uint (node, XML_NITERATIONS, &error_code);
            if (error_code == 1)
00697
              input->niterations = 1;
00698
00699
            else if (error_code)
00700
             {
                msg = gettext ("Bad iterations number");
00701
00702
                goto exit_on_error;
            }
00703
00704
00705
            // Obtaining best number
00706
            if (xmlHasProp (node, XML_NBEST))
00707
00708
                input->nbest = xml_node_get_uint (node,
     XML_NBEST, &error_code);
00709
              if (error_code || !input->nbest)
00710
                {
00711
                   msg = gettext ("Invalid best number");
00712
                    goto exit_on_error;
00713
00714
              }
00715
            else
              input->nbest = 1;
00716
00717
            // Obtaining tolerance
00718
00719
            if (xmlHasProp (node, XML_TOLERANCE))
00720
00721
                input->tolerance
                = xml_node_get_float (node, XML_TOLERANCE, &error_code);
if (error_code || input->tolerance < 0.)</pre>
00722
00723
00724
                 {
00725
                   msg = gettext ("Invalid tolerance");
00726
                    goto exit_on_error;
00727
                  }
00728
              }
00729
            else
00730
              input->tolerance = 0.;
00731
00732
            // Getting gradient method parameters
00733
            if (xmlHasProp (node, XML_NSTEPS))
00734
             {
                input->nsteps = xml_node_get_uint (node,
00735
     XML_NSTEPS, &error_code);
00736
              if (error_code || !input->nsteps)
00737
00738
                    msg = gettext ("Invalid steps number");
00739
                    goto exit_on_error;
00740
00741
                buffer = xmlGetProp (node, XML_GRADIENT_METHOD);
               if (!xmlStrcmp (buffer, XML_COORDINATES))
00743
                  input->gradient_method =
     GRADIENT_METHOD_COORDINATES;
00744
              else if (!xmlStrcmp (buffer, XML_RANDOM))
00745
                 {
                    input->gradient_method =
00746
     GRADIENT_METHOD_RANDOM;
00747
                  input->nestimates
00748
                      = xml_node_get_uint (node, XML_NESTIMATES, &error_code);
00749
                    if (error_code || !input->nestimates)
00750
                     {
00751
                       msg = gettext ("Invalid estimates number");
00752
                        goto exit_on_error;
00753
00754
                  }
00755
                else
00756
00757
                    msg = gettext ("Unknown method to estimate the gradient");
```

```
goto exit_on_error;
00759
00760
               xmlFree (buffer);
00761
               buffer = NULL;
00762
               if (xmlHasProp (node, XML_RELAXATION))
00763
                 {
00764
                   input->relaxation
00765
                      xml_node_get_float (node, XML_RELAXATION, &error_code);
00766
                   if (error_code || input->relaxation < 0.</pre>
00767
                       || input->relaxation > 2.)
                     {
00768
00769
                      msg = gettext ("Invalid relaxation parameter");
00770
                       goto exit on error;
00771
00772
                 }
               else
00773
                 input->relaxation = DEFAULT_RELAXATION;
00774
00775
             }
00776
           else
00777
             input->nsteps = 0;
00778
00779
00780
       \ensuremath{//} Reading the experimental data
00781
       for (child = node->children; child; child = child->next)
00782
00783
            if (xmlStrcmp (child->name, XML_EXPERIMENT))
00784
00785 #if DEBUG
           fprintf (stderr, "input_open: nexperiments=%u\n", input->nexperiments);
00786
00787 #endif
00788
           if (xmlHasProp (child, XML_NAME))
00789
             buffer = xmlGetProp (child, XML_NAME);
00790
           else
00791
             {
               00792
00793
00794
                         input->nexperiments + 1, gettext ("no data file name"));
00795
               msg = buffer2;
00796
               goto exit_on_error;
00797
00798 #if DEBUG
00799
           fprintf (stderr, "input_open: experiment=%s\n", buffer);
00800 #endif
00801
            input->weight = g_realloc (input->weight,
                                      (1 + input->nexperiments) * sizeof (double));
00802
00803
            if (xmlHasProp (child, XML_WEIGHT))
00804
00805
               input->weight[input->nexperiments]
                 = xml_node_get_float (child, XML_WEIGHT, &error_code);
00806
00807
               if (error code)
00808
                 {
                  00809
00810
00811
                   msg = buffer2;
00812
                   goto exit_on_error;
00813
                 }
00814
             }
00815
00816
             input->weight[input->nexperiments] = 1.;
00817 #if DEBUG
00818
           fprintf (stderr, "input_open: weight=%lg\n",
00819
                    input->weight[input->nexperiments]);
00820 #endif
       if (!input->nexperiments)
00821
00822
             input->ninputs = 0;
00823 #if DEBUG
00824
           fprintf (stderr, "input_open: template[0]\n");
00825 #endif
00826
           if (xmlHasProp (child, XML_TEMPLATE1))
             {
00828
               input->template[0]
00829
                  = (char **) g_realloc (input->template[0],
00830
                                        (1 + input->nexperiments) * sizeof (char *));
00831
               buffert[0] = (char *) xmlGetProp (child, template[0]);
00832 #if DEBUG
               fprintf (stderr, "input_open: experiment=%u template1=%s\n",
00833
00834
                        input->nexperiments, buffert[0]);
00835 #endif
00836
               if (!input->nexperiments)
00837
                 ++input->ninputs;
00838 #if DEBUG
00839
               fprintf (stderr, "input_open: ninputs=%u\n", input->ninputs);
00840 #endif
00841
             }
00842
           else
00843
00844
               snprintf (buffer2, 64, "%s %s: %s",
```

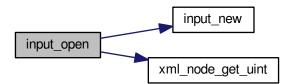
```
00845
                          gettext ("Experiment"), buffer, gettext ("no template"));
00846
               msg = buffer2;
00847
               goto exit_on_error;
00848
            for (i = 1; i < MAX_NINPUTS; ++i)</pre>
00849
00850
00851 #if DEBUG
00852
               fprintf (stderr, "input_open: template%u\n", i + 1);
00853 #endif
00854
               if (xmlHasProp (child, template[i]))
00855
00856
                    if (input->nexperiments && input->ninputs <= i)</pre>
00857
                       00858
00859
00860
                                 buffer, gettext ("bad templates number"));
00861
                       msg = buffer2;
                       while (i-- > 0)
00862
                        xmlFree (buffert[i]);
00863
00864
                       goto exit_on_error;
00865
00866
                    input->template[i] = (char **)
                     g_realloc (input->template[i],
00867
                                (1 + input->nexperiments) * sizeof (char *));
00868
00869
                   buffert[i] = (char *) xmlGetProp (child, template[i]);
00870 #if DEBUG
00871
                    fprintf (stderr, "input_open: experiment=%u template%u=%sn",
00872
                             input->nexperiments, i + 1,
00873
                            input->template[i][input->nexperiments]);
00874 #endif
00875
                   if (!input->nexperiments)
00876
                     ++input->ninputs;
00877 #if DEBUG
00878
                   fprintf (stderr, "input_open: ninputs=%u\n", input->ninputs);
00879 #endif
00880
00881
               else if (input->nexperiments && input->ninputs >= i)
                   snprintf (buffer2, 64, "%s %s: %s%u",
00883
00884
                             gettext ("Experiment"),
                             buffer, gettext ("no template"), i + 1);
00885
                   msq = buffer2;
00886
                   while (i-- > 0)
00887
00888
                     xmlFree (buffert[i]);
00889
                   goto exit_on_error;
00890
                 }
00891
               else
00892
                 break;
             }
00893
00894
            input->experiment
00895
              = g_realloc (input->experiment,
00896
                          (1 + input->nexperiments) * sizeof (char *));
00897
            input->experiment[input->nexperiments] = (char *) buffer;
00898
            for (i = 0; i < input->ninputs; ++i)
00899
             input->template[i][input->nexperiments] = buffert[i];
00900
            ++input->nexperiments;
00901 #if DEBUG
00902
            fprintf (stderr, "input_open: nexperiments=%u\n", input->nexperiments);
00903 #endif
00904
       if (!input->nexperiments)
00905
00906
00907
           msg = gettext ("No calibration experiments");
00908
           goto exit_on_error;
00909
00910
       buffer = NULL:
00911
00912
        // Reading the variables data
00913
       for (; child; child = child->next)
00915
            if (xmlStrcmp (child->name, XML_VARIABLE))
00916
               00917
00918
00919
                          input->nvariables + 1, gettext ("bad XML node"));
00920
               msg = buffer2;
00921
               goto exit_on_error;
00922
           if (xmlHasProp (child, XML_NAME))
buffer = xmlGetProp (child, XML_NAME);
00923
00924
00925
            else
00926
             {
               00927
00928
00929
                          input->nvariables + 1, gettext ("no name"));
               msq = buffer2;
00930
00931
               goto exit_on_error;
```

```
00933
           if (xmlHasProp (child, XML_MINIMUM))
00934
00935
              input->rangemin = g_realloc
              (input->rangemin, (1 + input->nvariables) * sizeof (double));
input->rangeminabs = g_realloc
00936
00937
                (input->rangeminabs, (1 + input->nvariables) * sizeof (double));
00939
              input->rangemin[input->nvariables]
00940
                = xml_node_get_float (child, XML_MINIMUM, &error_code);
00941
              if (error_code)
00942
                {
                  00943
00944
00945
                  msq = buffer2;
00946
                  goto exit_on_error;
00947
              if (xmlHasProp (child, XML_ABSOLUTE_MINIMUM))
00948
00949
                  input->rangeminabs[input->nvariables]
00951
                    = xml_node_get_float (child,
     XML_ABSOLUTE_MINIMUM, &error_code);
00952
                  if (error_code)
00953
                     00954
00955
                               buffer, gettext ("bad absolute minimum"));
00956
00957
                     msg = buffer2;
                     goto exit_on_error;
00958
00959
00960
                }
00961
              else
00962
                input->rangeminabs[input->nvariables] = -G_MAXDOUBLE;
00963
               if (input->rangemin[input->nvariables]
00964
                  < input->rangeminabs[input->nvariables])
00965
                  00966
00967
                           buffer, gettext ("minimum range not allowed"));
                  msg = buffer2;
00969
00970
                  goto exit_on_error;
00971
                }
00972
00973
          else
00974
              00975
00976
00977
              msq = buffer2;
00978
              goto exit_on_error;
00979
00980
           if (xmlHasProp (child, XML_MAXIMUM))
            {
00982
              input->rangemax = g_realloc
00983
                 (input->rangemax, (1 + input->nvariables) \star sizeof (double));
              input->rangemaxabs = g_realloc
00984
              (input->rangemaxabs, (1 + input->nvariables) * sizeof (double));
input->rangemax[input->nvariables]
00985
00986
                = xml_node_get_float (child, XML_MAXIMUM, &error_code);
00988
              if (error_code)
00989
                  00990
00991
                  msg = buffer2;
00992
00993
                  goto exit_on_error;
00994
00995
              if (xmlHasProp (child, XML_ABSOLUTE_MAXIMUM))
00996
00997
                  input->rangemaxabs[input->nvariables]
00998
                    = xml_node_get_float (child,
     XML_ABSOLUTE_MAXIMUM, &error_code);
00999
                  if (error_code)
01000
                      01001
01002
                               buffer, gettext ("bad absolute maximum"));
01003
01004
                     msq = buffer2;
01005
                     goto exit_on_error;
01006
01007
01008
              else
01009
                input->rangemaxabs[input->nvariables] = G MAXDOUBLE;
              if (input->rangemax[input->nvariables]
01010
                  > input->rangemaxabs[input->nvariables])
01012
                  snprintf (buffer2, 64, "%s %s: %s",
01013
01014
                           gettext ("Variable"),
                           buffer, gettext ("maximum range not allowed"));
01015
01016
                  msq = buffer2;
```

```
goto exit_on_error;
01018
01019
             }
           else
01020
01021
            {
               snprintf (buffer2, 64, "%s %s: %s",
01022
                         gettext ("Variable"), buffer, gettext ("no maximum range"));
01023
01024
                msg = buffer2;
01025
               goto exit_on_error;
01026
01027
            if (input->rangemax[input->nvariables]
01028
               < input->rangemin[input->nvariables])
01029
             {
01030
               snprintf (buffer2, 64, "%s %s: %s",
01031
                         gettext ("Variable"), buffer, gettext ("bad range"));
                msg = buffer2;
01032
01033
               goto exit_on_error;
              }
01034
            input->precision = g_realloc
01035
01036
              (input->precision, (1 + input->nvariables) * sizeof (unsigned int));
01037
              (xmlHasProp (child, XML_PRECISION))
01038
01039
                input->precision[input->nvariables]
                = xml_node_get_uint (child, XML_PRECISION, &error_code);
if (error_code || input->precision[input->
01040
01041
     nvariables] >= NPRECISIONS)
01042
                   01043
01044
                             buffer, gettext ("bad precision"));
01045
01046
                   msg = buffer2;
01047
                   goto exit_on_error;
01048
01049
             }
01050
           else
01051
             input->precision[input->nvariables] =
     DEFAULT_PRECISION;
01052
           if (input->algorithm == ALGORITHM_SWEEP)
01053
             {
01054
                if (xmlHasProp (child, XML_NSWEEPS))
01055
01056
                   input->nsweeps = (unsigned int *)
01057
                     g_realloc (input->nsweeps,
01058
                                (1 + input->nvariables) * sizeof (unsigned int));
                    input->nsweeps[input->nvariables]
01059
01060
                      = xml_node_get_uint (child, XML_NSWEEPS, &error_code);
01061
                    if (error_code || !input->nsweeps[input->
     nvariables])
01062
                       01063
01065
                                 buffer, gettext ("bad sweeps"));
01066
                       msg = buffer2;
01067
                       goto exit_on_error;
01068
01069
                  }
01070
               else
01071
                 {
                   01072
01073
                             buffer, gettext ("no sweeps number"));
01074
01075
                   msq = buffer2;
01076
                   goto exit_on_error;
01077
01078 #if DEBUG
01079
               fprintf (stderr, "input_open: nsweeps=%u nsimulations=%u\n",
01080
                         input->nsweeps[input->nvariables],
      input->nsimulations);
01081 #endif
01082
01083
            if (input->algorithm == ALGORITHM_GENETIC)
01084
01085
                \ensuremath{//} Obtaining bits representing each variable
01086
                if (xmlHasProp (child, XML_NBITS))
01087
                 {
                   input->nbits = (unsigned int *)
01088
01089
                     g_realloc (input->nbits,
01090
                                (1 + input->nvariables) * sizeof (unsigned int));
01091
                    i = xml_node_get_uint (child, XML_NBITS, &error_code);
01092
                    if (error_code || !i)
01093
01094
                       snprintf (buffer2, 64, "%s %s: %s",
01095
                                 gettext ("Variable"),
01096
                                 buffer, gettext ("invalid bits number"));
                       msg = buffer2;
01097
01098
                       goto exit_on_error;
01099
```

```
input->nbits[input->nvariables] = i;
01101
01102
                else
01103
                 {
                   01104
01105
                              buffer, gettext ("no bits number"));
01106
01107
                    msg = buffer2;
01108
                    goto exit_on_error;
01109
01110
01111
            else if (input->nsteps)
01112
01113
                input->step = (double *)
01114
                  g_realloc (input->step, (1 + input->nvariables) * sizeof (double));
01115
                input->step[input->nvariables]
                = xml_node_get_float (child, XML_STEP, &error_code);
if (error_code || input->step[input->nvariables] < 0.)
01116
01117
01118
01119
                    snprintf (buffer2, 64, "%s %s: %s",
01120
                              gettext ("Variable"),
01121
                              buffer, gettext ("bad step size"));
                   msq = buffer2;
01122
01123
                    goto exit_on_error;
01124
                  }
01125
01126
            input->label = g_realloc
01127
              (input->label, (1 + input->nvariables) * sizeof (char *));
01128
            input->label[input->nvariables] = (char *) buffer;
01129
            ++input->nvariables:
01130
01131
        if (!input->nvariables)
01132
01133
            msg = gettext ("No calibration variables");
01134
            goto exit_on_error;
01135
       buffer = NULL;
01136
01137
01138
        // Getting the working directory
01139
        input->directory = g_path_get_dirname (filename);
01140
        input->name = g_path_get_basename (filename);
01141
       // Closing the XML document
01142
01143
       xmlFreeDoc (doc);
01144
01145 #if DEBUG
01146 fprintf (stderr, "input_open: end\n");
01147 #endif
01148
       return 1;
01149
01150 exit_on_error:
01151 xmlFree (buffer);
01152 xmlFreeDoc (doc);
       xmlFreeDoc (doc);
01153 show_error (msg);
01154
        input_free ();
01155 #if DEBUG
       fprintf (stderr, "input_open: end\n");
01157 #endif
       return 0;
01158
01159 }
```

Here is the call graph for this function:



5.5.2.16 void input_save (char * filename)

Function to save the input file.

Parameters

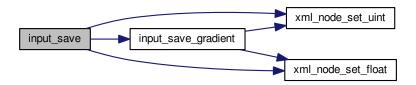
filename Input file name.

Definition at line 2670 of file mpcotool.c.

```
02671 {
02672
         unsigned int i, j;
02673
         char *buffer;
02674
         xmlDoc *doc;
02675
         xmlNode *node, *child;
02676
         GFile *file, *file2;
02677
         // Getting the input file directory
02678
02679
         input->name = g_path_get_basename (filename);
          input->directory = g_path_get_dirname (filename);
02680
         file = g_file_new_for_path (input->directory);
02682
02683
          // Opening the input file
02684
         doc = xmlNewDoc ((const xmlChar *) "1.0");
02685
02686
         // Setting root XML node
02687
         node = xmlNewDocNode (doc, 0, XML_CALIBRATE, 0);
02688
         xmlDocSetRootElement (doc, node);
02689
02690
         // Adding properties to the root XML node
         if (xmlStrcmp ((const xmlChar *) input->result, result_name))
   xmlSetProp (node, XML_RESULT, (xmlChar *) input->result);
02691
02692
02693
          if (xmlStrcmp ((const xmlChar *) input->variables,
       variables_name))
02694
           xmlSetProp (node, XML_VARIABLES, (xmlChar *) input->
      variables);
02695 file2 = g_file_new_for_path (input->simulator);
02696
         buffer = g_file_get_relative_path (file, file2);
02697
         g_object_unref (file2);
          xmlSetProp (node, XML_SIMULATOR, (xmlChar *) buffer);
02699
         g_free (buffer);
02700
          if (input->evaluator)
02701
           {
02702
              file2 = g_file_new_for_path (input->evaluator);
02703
              buffer = g_file_get_relative_path (file, file2);
02704
              g_object_unref (file2);
02705
              if (xmlStrlen ((xmlChar *) buffer))
02706
                xmlSetProp (node, XML_EVALUATOR, (xmlChar *) buffer);
              g_free (buffer);
02707
02708
02709
         if (input->seed != DEFAULT_RANDOM_SEED)
02710
           xml_node_set_uint (node, XML_SEED, input->seed);
02711
02712
         // Setting the algorithm
02713
         buffer = (char *) g_malloc (64);
         switch (input->algorithm)
02714
02715
02716
           case ALGORITHM_MONTE_CARLO:
02717
              xmlSetProp (node, XML_ALGORITHM, XML_MONTE_CARLO);
02718
              snprintf (buffer, 64, "%u", input->nsimulations);
              xmlSetProp (node, XML_NSIMULATIONS, (xmlChar *) buffer);
02719
              snprintf (buffer, 64, "%u", input->niterations);
xmlSetProp (node, XML_NITERATIONS, (xmlChar *) buffer);
02720
02721
              snprintf (buffer, 64, "%.31g", input->tolerance);
xmlSetProp (node, XML_TOLERANCE, (xmlChar *) buffer);
02722
02723
02724
              snprintf (buffer, 64, "%u", input->nbest);
              xmlSetProp (node, XML_NBEST, (xmlChar *) buffer);
02725
02726
              input_save_gradient (node);
02727
              break:
           case ALGORITHM_SWEEP:
02728
              xmlSetProp (node, XML_ALGORITHM, XML_SWEEP);
02729
02730
              snprintf (buffer, 64, "%u", input->niterations);
02731
              xmlSetProp (node, XML_NITERATIONS, (xmlChar *) buffer);
              xmlSetProp (node, XML_TOLERANCE, (xmlChar *) buffer);
xmlSetProp (node, XML_TOLERANCE, (xmlChar *) buffer);
snprintf (buffer, 64, "%u", input->nbest);
xmlSetProp (node, XML_NBEST, (xmlChar *) buffer);
02732
02733
02734
02735
02736
               input_save_gradient (node);
02737
02738
            default:
              xmlSetProp (node, XML_ALGORITHM, XML_GENETIC);
snprintf (buffer, 64, "%u", input->nsimulations);
xmlSetProp (node, XML_NPOPULATION, (xmlChar *) buffer);
02739
02740
02741
02742
              snprintf (buffer, 64, "%u", input->niterations);
02743
              xmlSetProp (node, XML_NGENERATIONS, (xmlChar *) buffer);
02744
              snprintf (buffer, 64, "%.31g", input->mutation_ratio);
              xmlSetProp (node, XML_MUTATION, (xmlChar *) buffer);
snprintf (buffer, 64, "%.31g", input->reproduction_ratio);
xmlSetProp (node, XML_REPRODUCTION, (xmlChar *) buffer);
02745
02746
              snprintf (buffer, 64, "%.31g", input->adaptation_ratio);
```

```
xmlSetProp (node, XML_ADAPTATION, (xmlChar *) buffer);
02750
02751
02752
        g_free (buffer);
02753
02754
        // Setting the experimental data
02755
        for (i = 0; i < input->nexperiments; ++i)
02756
02757
             child = xmlNewChild (node, 0, XML_EXPERIMENT, 0);
            xmlSetProp (child, XML_NAME, (xmlChar *) input->experiment[i]);
if (input->weight[i] != 1.)
02758
02759
              xml_node_set_float (child, XML_WEIGHT, input->
02760
      weight[i]);
02761
            for (j = 0; j < input->ninputs; ++j)
02762
              xmlSetProp (child, template[j], (xmlChar *) input->template[j][i]);
02763
02764
02765
        // Setting the variables data
        for (i = 0; i < input->nvariables; ++i)
02767
        {
            child = xmlNewChild (node, 0, XML_VARIABLE, 0);
xmlSetProp (child, XML_NAME, (xmlChar *) input->label[i]);
02768
02769
            xml_node_set_float (child, XML_MINIMUM, input->
02770
      rangemin[i]);
02771
            if (input->rangeminabs[i] != -G_MAXDOUBLE)
              xml_node_set_float (child, XML_ABSOLUTE_MINIMUM,
02772
      input->rangeminabs[i]);
02773
            xml_node_set_float (child, XML_MAXIMUM, input->
      rangemax[i]);
           if (input->rangemaxabs[i] != G_MAXDOUBLE)
02774
             xml_node_set_float (child, XML_ABSOLUTE_MAXIMUM,
02775
      input->rangemaxabs[i]);
02776
          if (input->precision[i] != DEFAULT_PRECISION)
02777
              xml_node_set_uint (child, XML_PRECISION,
      input->precision[i]);
           if (input->algorithm == ALGORITHM_SWEEP)
02778
02779
              xml_node_set_uint (child, XML_NSWEEPS, input->
     nsweeps[i]);
        else if (input->algorithm == ALGORITHM_GENETIC)
02780
02781
              xml_node_set_uint (child, XML_NBITS, input->
      nbits[i]);
02782
02783
02784
        // Saving the XML file
02785
       xmlSaveFormatFile (filename, doc, 1);
02786
02787
        // Freeing memory
02788
       xmlFreeDoc (doc);
02789 }
```

Here is the call graph for this function:



5.5.2.17 void input_save_gradient (xmlNode * node)

Function to save the gradient based method data in a XML node.

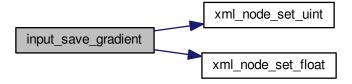
Parameters

node XML node.

Definition at line 2644 of file mpcotool.c.

```
02645 {
02646
        if (input->nsteps)
02647
          {
02648
            xml_node_set_uint (node, XML_NSTEPS, input->
nsteps);
02649 if (input->relaxation != DEFAULT_RELAXATION)
              xml_node_set_float (node, XML_RELAXATION,
02650
      input->relaxation);
          switch (input->gradient_method)
02651
02652
              case GRADIENT_METHOD_COORDINATES:
02653
               xmlSetProp (node, XML_GRADIENT_METHOD,
02654
XML_COORDINATES);
02655 break;
02656
               default:
               xmlSetProp (node, XML_GRADIENT_METHOD, XML_RANDOM);
xml_node_set_uint (node, XML_NESTIMATES,
02657
02658
input->nestimates);
02659 }
             }
02660
          }
02661 }
```

Here is the call graph for this function:



5.5.2.18 int main (int argn, char ** argc)

Main function.

Parameters

argn	Arguments number.
argc	Arguments pointer.

Returns

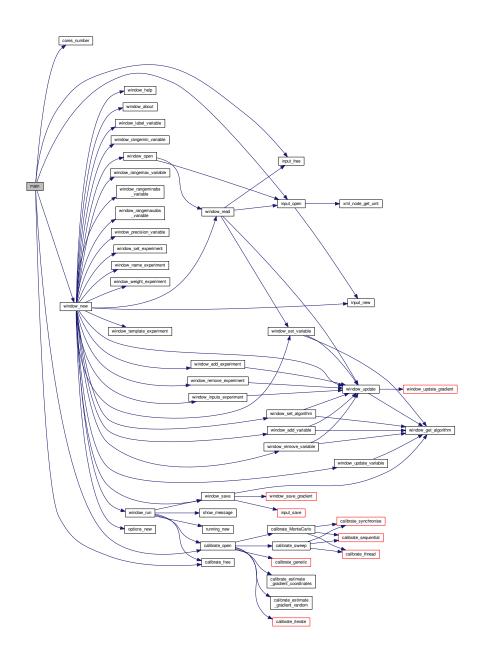
0 on success, >0 on error.

Definition at line 4728 of file mpcotool.c.

```
04729 {
04730 #if HAVE_GTK
04731    char *buffer;
04732 #endif
04733
04734    // Starting pseudo-random numbers generator
04735    calibrate->rng = gsl_rng_alloc (gsl_rng_taus2);
04736    calibrate->seed = DEFAULT_RANDOM_SEED;
04737
```

```
// Allowing spaces in the XML data file
04739
        xmlKeepBlanksDefault (0);
04740
04741
        // Starting MPI
04742 #if HAVE MPI
04743
        MPI_Init (&argn, &argc);
04744
        MPI_Comm_size (MPI_COMM_WORLD, &ntasks);
04745
        MPI_Comm_rank (MPI_COMM_WORLD, &calibrate->mpi_rank);
04746
        printf ("rank=%d tasks=%d\n", calibrate->mpi_rank, ntasks);
04747 #else
04748
       ntasks = 1:
04749 #endif
04750
04751 #if HAVE_GTK
04752
04753
        // Getting threads number
04754
       nthreads_gradient = nthreads = cores_number ();
04755
04756
       // Setting local language and international floating point numbers notation
04757
       setlocale (LC_ALL, "");
        setlocale (LC_NUMERIC, "C");
04758
04759
        window->application_directory = g_get_current_dir ();
04760 buffer = g_build_filename (window->application_directory,
     LOCALE_DIR, NULL);
04761
        bindtextdomain (PROGRAM_INTERFACE, buffer);
04762
        bind_textdomain_codeset (PROGRAM_INTERFACE, "UTF-8");
04763
        textdomain (PROGRAM_INTERFACE);
04764
04765
       // Initing GTK+
       gtk_disable_setlocale ();
04766
04767
       gtk init (&argn, &argc);
04768
04769
       // Opening the main window
04770
       window_new ();
04771
       gtk_main ();
04772
04773
       // Freeing memory
04774
       input_free ();
04775
        g_free (buffer);
04776
        gtk_widget_destroy (GTK_WIDGET (window->window));
04777
        g_free (window->application_directory);
04778
04779 #else
04780
04781
        // Checking syntax
04782
        if (!(argn == 2 || (argn == 4 && !strcmp (argc[1], "-nthreads"))))
04783
           printf ("The syntax is:\nmpcotoolbin [-nthreads x] data_file n");
04784
04785
            return 1:
04786
04787
04788
        // Getting threads number
04789
        if (argn == 2)
04790
         nthreads_gradient = nthreads = cores_number ();
04791
        else
04792
04793
            nthreads_gradient = nthreads = atoi (argc[2]);
04794
            if (!nthreads)
04795
                printf ("Bad threads number\n");
04796
04797
                return 2;
04798
04799
04800
       printf ("nthreads=%u\n", nthreads);
04801
04802
        // Making calibration
04803
        if (input_open (argc[argn - 1]))
  calibrate_open ();
04804
04805
04806
       // Freeing memory
04807
       calibrate_free ();
04808
04809 #endif
04810
        // Closing MPI
04811
04812 #if HAVE_MPI
04813
       MPI_Finalize ();
04814 #endif
04815
       // Freeing memory
04816
       gsl_rng_free (calibrate->rng);
04817
       // Closing
04819
04820
        return 0;
04821 }
```

Here is the call graph for this function:



5.5.2.19 void show_error (char * msg)

Function to show a dialog with an error message.

Parameters

msg	Error message.

Definition at line 256 of file mpcotool.c.

```
00257 {
00258     show_message (gettext ("ERROR!"), msg, ERROR_TYPE);
00259 }
```

Here is the call graph for this function:



5.5.2.20 void show_message (char * title, char * msg, int type)

Function to show a dialog with a message.

Parameters

title	Title.
msg	Message.
type	Message type.

Definition at line 226 of file mpcotool.c.

```
00227 {
00228 #if HAVE_GTK
00229
        GtkMessageDialog *dlg;
00230
00231
        // Creating the dialog
       dlg = (GtkMessageDialog *) gtk_message_dialog_new
  (window->window, GTK_DIALOG_MODAL, type, GTK_BUTTONS_OK, "%s", msg);
00232
00233
00234
00235
        // Setting the dialog title
00236
        gtk_window_set_title (GTK_WINDOW (dlg), title);
00237
00238
00239
        // Showing the dialog and waiting response
        gtk_dialog_run (GTK_DIALOG (dlg));
00240
00241
        // Closing and freeing memory
00242
       gtk_widget_destroy (GTK_WIDGET (dlg));
00243
00244 #else
       printf ("%s: %s\n", title, msg);
00245
00246 #endif
00247 }
```

5.5.2.21 int window_get_algorithm ()

Function to get the stochastic algorithm number.

Returns

Stochastic algorithm number.

Definition at line 2887 of file mpcotool.c.

5.5.2.22 int window_get_gradient ()

Function to get the gradient base method number.

Returns

Gradient base method number.

Definition at line 2903 of file mpcotool.c.

5.5.2.23 int window_read (char * filename)

Function to read the input data of a file.

Parameters

```
filename File name.
```

Returns

1 on succes, 0 on error.

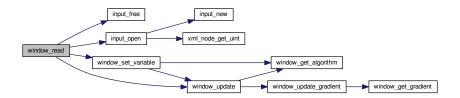
Definition at line 3908 of file mpcotool.c.

```
03909 {
        unsigned int i;
03911
        char *buffer;
03912 #if DEBUG
03913
       fprintf (stderr, "window_read: start\n");
03914 #endif
03915
03916
       // Reading new input file
03917
       input_free ();
03918
       if (!input_open (filename))
03919
          return 0;
03920
       // Setting GTK+ widgets data
03921
03922
       gtk_entry_set_text (window->entry_result, input->result);
        gtk_entry_set_text (window->entry_variables, input->
03924
simulator, NULL);

03925 qtk file
       buffer = g_build_filename (input->directory, input->
        gtk_file_chooser_set_filename (GTK_FILE_CHOOSER
03926
                                        (window->button simulator), buffer);
03927
        g_free (buffer);
03928
        gtk_toggle_button_set_active (GTK_TOGGLE_BUTTON (window->check_evaluator),
03929
                                       (size_t) input->evaluator);
03930
        if (input->evaluator)
03931
           buffer = g_build_filename (input->directory, input->
03932
      evaluator, NULL);
03933
            gtk_file_chooser_set_filename (GTK_FILE_CHOOSER
03934
                                            (window->button_evaluator), buffer);
03935
            g_free (buffer);
03936
03937
        gtk_toggle_button_set_active
          (GTK_TOGGLE_BUTTON (window->button_algorithm[input->
03938
     algorithm]), TRUE);
       switch (input->algorithm)
03939
03940
03941
          case ALGORITHM MONTE CARLO:
03942
            gtk_spin_button_set_value (window->spin_simulations,
03943
                                        (gdouble) input->nsimulations);
03944
          case ALGORITHM_SWEEP:
```

```
03945
            gtk_spin_button_set_value (window->spin_iterations,
03946
                                        (gdouble) input->niterations);
03947
            gtk_spin_button_set_value (window->spin_bests, (gdouble)
      input->nbest);
03948
           gtk_spin_button_set_value (window->spin_tolerance,
      input->tolerance);
03949
           gtk_toggle_button_set_active (GTK_TOGGLE_BUTTON (window->
      check_gradient),
03950
                                          input->nsteps);
03951
            if (input->nsteps)
03952
                gtk_toggle_button_set active
03953
03954
                  (GTK_TOGGLE_BUTTON (window->button_gradient
03955
                                       [input->gradient_method]), TRUE);
03956
                gtk_spin_button_set_value (window->spin_steps,
03957
                                            (gdouble) input->nsteps);
03958
                gtk_spin_button_set_value (window->spin_relaxation,
03959
                                            (gdouble) input->relaxation);
03960
                switch (input->gradient_method)
03961
03962
                  case GRADIENT_METHOD_RANDOM:
03963
                    gtk_spin_button_set_value (window->spin_estimates,
03964
                                                (gdouble) input->nestimates);
03965
                  }
03966
              }
03967
           break;
03968
          default:
03969
           gtk_spin_button_set_value (window->spin_population,
03970
                                        (gdouble) input->nsimulations);
03971
            gtk_spin_button_set_value (window->spin_generations,
03972
                                        (gdouble) input->niterations);
03973
            gtk_spin_button_set_value (window->spin_mutation, input->
      mutation_ratio);
03974
            gtk_spin_button_set_value (window->spin_reproduction,
03975
                                        input->reproduction_ratio);
03976
            gtk_spin_button_set_value (window->spin_adaptation,
03977
                                        input->adaptation_ratio);
03978
03979
        g_signal_handler_block (window->combo_experiment, window->
      id_experiment);
03980
        g_signal_handler_block (window->button_experiment,
03981
                                window->id_experiment_name);
        gtk_combo_box_text_remove_all (window->combo_experiment);
03982
03983
        for (i = 0; i < input->nexperiments; ++i)
          gtk_combo_box_text_append_text (window->combo_experiment,
03984
03985
                                          input->experiment[i]);
03986
        g_signal_handler_unblock
03987
          (window->button_experiment, window->
      id experiment name);
03988
        g signal handler unblock (window->combo experiment,
      window->id_experiment);
03989
      gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_experiment), 0);
03990
        g_signal_handler_block (window->combo_variable, window->
      id variable);
        g_signal_handler_block (window->entry_variable, window->
03991
      id variable label);
03992
      gtk_combo_box_text_remove_all (window->combo_variable);
            (i = 0; i < input->nvariables; ++i)
03993
03994
          gtk_combo_box_text_append_text (window->combo_variable,
      input->label[i]);
03995
        g_signal_handler_unblock (window->entry_variable, window->
      id variable label);
03996
        g_signal_handler_unblock (window->combo_variable, window->
      id_variable);
03997
        gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_variable), 0);
03998
       window_set_variable ();
03999
       window_update ();
04000
04001 #if DEBUG
       fprintf (stderr, "window_read: end\n");
04003 #endif
04004
       return 1;
04005 }
```

Here is the call graph for this function:



5.5.2.24 int window_save ()

Function to save the input file.

Returns

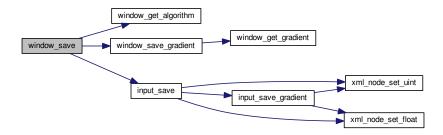
1 on OK, 0 on Cancel.

Definition at line 2951 of file mpcotool.c.

```
02952 {
02953
         char *buffer;
02954
        GtkFileChooserDialog *dlg;
02955
02956 #if DEBUG
02957
        fprintf (stderr, "window_save: start\n");
02958 #endif
02959
02960
         // Opening the saving dialog
02961
        dlg = (GtkFileChooserDialog *)
02962
           gtk_file_chooser_dialog_new (gettext ("Save file"),
02963
                                            window->window,
02964
                                            GTK_FILE_CHOOSER_ACTION_SAVE,
02965
                                            gettext ("_Cancel"),
02966
                                            GTK_RESPONSE_CANCEL,
02967
                                            gettext ("_OK"), GTK_RESPONSE_OK, NULL);
        gtk_file_chooser_set_do_overwrite_confirmation (GTK_FILE_CHOOSER (dlg), TRUE);
buffer = g_build_filename (input->directory, input->name, NULL);
02968
02969
02970
        gtk_file_chooser_set_filename (GTK_FILE_CHOOSER (dlg), buffer);
02971
        g_free (buffer);
02972
02973
         // If OK response then saving
02974
         if (gtk_dialog_run (GTK_DIALOG (dlg)) == GTK_RESPONSE_OK)
02975
02976
02977
             // Adding properties to the root XML node
02978
             input->simulator = gtk_file_chooser_get_filename
                (GTK_FILE_CHOOSER (window->button_simulator));
02979
02980
             if (gtk_toggle_button_get_active
  (GTK_TOGGLE_BUTTON (window->check_evaluator)))
02981
                input->evaluator = gtk_file_chooser_get_filename
  (GTK_FILE_CHOOSER (window->button_evaluator));
02982
02983
02984
02985
               input->evaluator = NULL;
02986
             input->result
02987
                = (char *) xmlStrdup ((const xmlChar *)
02988
                                        gtk_entry_get_text (window->entry_result));
02989
             input->variables
02990
                = (char *) xmlStrdup ((const xmlChar *)
02991
                                        gtk_entry_get_text (window->entry_variables));
02992
02993
             // Setting the algorithm
02994
             switch (window_get_algorithm ())
02995
02996
                case ALGORITHM_MONTE_CARLO:
02997
                  input->algorithm = ALGORITHM_MONTE_CARLO;
                  input->nsimulations
02998
02999
                  = gtk_spin_button_get_value_as_int (window->spin_simulations);
input->niterations
03000
03001
                    = gtk_spin_button_get_value_as_int (window->spin_iterations);
03002
                  input->tolerance = gtk_spin_button_get_value (window->
```

```
spin_tolerance);
03003
                input->nbest = gtk_spin_button_get_value_as_int (window->
      spin_bests);
03004
                window_save_gradient ();
03005
                break;
              case ALGORITHM_SWEEP:
03006
               input->algorithm = ALGORITHM_SWEEP;
03008
                input->niterations
03009
                  = gtk_spin_button_get_value_as_int (window->spin_iterations);
03010
                input->tolerance = gtk_spin_button_get_value (window->
      spin_tolerance);
03011
                input->nbest = gtk_spin_button_get_value_as_int (window->
     spin bests);
03012
                window_save_gradient ();
03013
                break;
03014
              default:
                input->algorithm = ALGORITHM_GENETIC;
03015
               input->nsimulations
03016
03017
                  = gtk_spin_button_get_value_as_int (window->spin_population);
03018
                input->niterations
03019
                   -
= gtk_spin_button_get_value_as_int (window->spin_generations);
03020
03021
                  = gtk_spin_button_get_value (window->spin_mutation);
03022
                input->reproduction ratio
03023
                  = gtk_spin_button_get_value (window->spin_reproduction);
03024
                input->adaptation_ratio
03025
                   = gtk_spin_button_get_value (window->spin_adaptation);
03026
03027
              }
03028
03029
            // Saving the XML file
03030
            buffer = gtk_file_chooser_get_filename (GTK_FILE_CHOOSER (dlg));
03031
            input_save (buffer);
03032
            // Closing and freeing memory
g_free (buffer);
03033
03034
            gtk_widget_destroy (GTK_WIDGET (dlg));
03035
03036 #if DEBUG
03037
            fprintf (stderr, "window_save: end\n");
03038 #endif
03039
            return 1;
          }
03040
03041
03042
       // Closing and freeing memory
03043
        gtk_widget_destroy (GTK_WIDGET (dlg));
03044 #if DEBUG
03045
       fprintf (stderr, "window_save: end\n");
03046 #endif
03047
        return 0:
03048 }
```

Here is the call graph for this function:



5.5.2.25 void window_template_experiment (void * data)

Function to update the experiment i-th input template in the main window.

Parameters

data Callback data (i-th input template).

Definition at line 3544 of file mpcotool.c.

```
03545 {
03546
        unsigned int i, j;
         char *buffer;
03548
        GFile *file1, *file2;
03549 #if DEBUG
03550
        fprintf (stderr, "window_template_experiment: start\n");
03551 #endif
03552
        i = (size t) data;
         j = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_experiment));
03553
03554
        file1
03555
          = gtk_file_chooser_get_file (GTK_FILE_CHOOSER (window->button_template[i]));
        file2 = g_file_new_for_path (input->directory);
buffer = g_file_get_relative_path (file2, file1);
input->template[i][j] = (char *) xmlStrdup ((xmlChar *) buffer);
03556
03557
03558
03559
        g_free (buffer);
03560
        g_object_unref (file2);
03561
         g_object_unref (file1);
03562 #if DEBUG
03563 fprintf (stderr, "window_template_experiment: end\n");
03564 #endif
03565 }
```

5.5.2.26 double xml_node_get_float (xmlNode * node, const xmlChar * prop, int * error_code)

Function to get a floating point number of a XML node property.

Parameters

node	XML node.
prop	XML property.
error_code	Error code.

Returns

Floating point number value.

Definition at line 336 of file mpcotool.c.

```
00337 {
00338
        double x = 0.;
        xmlChar *buffer;
buffer = xmlGetProp (node, prop);
00339
00340
00341
        if (!buffer)
00342
          *error_code = 1;
00343
        else
00344
00345
            if (sscanf ((char *) buffer, "%lf", &x) != 1)
00346
              *error_code = 2;
            else
00348
               *error_code = 0;
00349
             xmlFree (buffer);
00350
00351
        return x;
00352 }
```

5.5.2.27 int xml_node_get_int (xmlNode * node, const xmlChar * prop, int * error_code)

Function to get an integer number of a XML node property.

Parameters

node	XML node.
prop	XML property.
error_code	Error code.

Returns

Integer number value.

Definition at line 274 of file mpcotool.c.

```
00275 {
00276
         int i = 0;
         xmlChar *buffer;
buffer = xmlGetProp (node, prop);
00277
00278
         if (!buffer)
  *error_code = 1;
00279
00280
00281
         else
         {
   if (sscanf ((char *) buffer, "%d", &i) != 1)
     *error_code = 2;
   else
00282
00283
00284
00285
00286
                *error_code = 0;
         xmlFree (buffer);
}
00287
00288 } 00289 return i; 00290 }
```

5.5.2.28 int xml_node_get_uint (xmlNode * node, const xmlChar * prop, int * error_code)

Function to get an unsigned integer number of a XML node property.

Parameters

node	XML node.
prop	XML property.
error_code	Error code.

Returns

Unsigned integer number value.

Definition at line 305 of file mpcotool.c.

```
00306 {
00307
         unsigned int i = 0;
        xmlChar *buffer;
buffer = xmlGetProp (node, prop);
00308
00309
        if (!buffer)
  *error_code = 1;
00310
00311
00312
         else
         {
  if (sscanf ((char *) buffer, "%u", &i) != 1)
    *error code = ?*
00313
00314
00315
                *error_code = 2;
00316
           else
             *error_code = 0;
xmlFree (buffer);
00317
00318
00319
00320 return i;
00321 }
```

5.5.2.29 void xml_node_set_float (xmlNode * node, const xmlChar * prop, double value)

Function to set a floating point number in a XML node property.

Parameters

node	XML node.
prop	XML property.
value	Floating point number value.

Definition at line 403 of file mpcotool.c.

5.5.2.30 void xml_node_set_int (xmlNode * node, const xmlChar * prop, int value)

Function to set an integer number in a XML node property.

Parameters

node	XML node.
prop	XML property.
value	Integer number value.

Definition at line 365 of file mpcotool.c.

5.5.2.31 void xml_node_set_uint (xmlNode * node, const xmlChar * prop, unsigned int value)

Function to set an unsigned integer number in a XML node property.

Parameters

node	XML node.
prop	XML property.
value	Unsigned integer number value.

Definition at line 384 of file mpcotool.c.

5.5.3 Variable Documentation

5.5.3.1 const char* format[NPRECISIONS]

Initial value:

```
= {
    "%.11g", "%.21g", "%.31g", "%.41g", "%.51g", "%.61g", "%.71g", "%.81g",
    "%.91g", "%.101g", "%.111g", "%.121g", "%.131g", "%.141g", "%.151g"
}
```

Array of C-strings with variable formats.

Definition at line 117 of file mpcotool.c.

5.5.3.2 const double precision[NPRECISIONS]

Initial value:

```
= {
   1., 0.1, 0.01, 1e-3, 1e-4, 1e-5, 1e-6, 1e-7, 1e-8, 1e-9, 1e-10, 1e-11, 1e-12, 1e-13, 1e-14
}
```

Array of variable precisions.

Definition at line 122 of file mpcotool.c.

5.5.3.3 const xmlChar* template[MAX_NINPUTS]

Initial value:

Array of xmlChar strings with template labels.

Definition at line 110 of file mpcotool.c.

```
00002 MPCOTool: a software to make calibrations of empirical parameters.
00003
00004 AUTHORS: Javier Burguete and Boria Latorre.
00005
00006 Copyright 2012-2015, AUTHORS.
00007
00008 Redistribution and use in source and binary forms, with or without modification,
00009 are permitted provided that the following conditions are met:
00010
00011
          1. Redistributions of source code must retain the above copyright notice,
00012
               this list of conditions and the following disclaimer.
00013
00014
          2. Redistributions in binary form must reproduce the above copyright notice,
               this list of conditions and the following disclaimer in the
00015
00016
               documentation and/or other materials provided with the distribution.
00017
00018 THIS SOFTWARE IS PROVIDED BY AUTHORS "AS IS" AND ANY EXPRESS OR IMPLIED
00019 WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF
00020 MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT
00021 SHALL AUTHORS OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL,
00022 SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, 00023 PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR
00024 BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN
00025 CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING
00026 IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY
00027 OF SUCH DAMAGE.
00028 */
00029
00036 #define _GNU_SOURCE
00037 #include "config.h"
00038 #include <stdio.h>
00039 #include <stdlib.h>
00040 #include <string.h>
00041 #include <math.h>
00042 #include <unistd.h>
00043 #include <locale.h>
00044 #include <gsl/gsl_rng.h>
00045 #include <libxml/parser.h>
00046 #include <libintl.h>
00047 #include <glib.h>
00048 #include <glib/gstdio.h>
00049 #ifdef G_OS_WIN32
00050 #include <windows.h>
```

```
00051 #elif (!__BSD_VISIBLE)
00052 #include <alloca.h>
00053 #endif
00054 #if HAVE MPI
00055 #include <mpi.h>
00056 #endif
00057 #include "genetic/genetic.h"
00058 #include "mpcotool.h"
00059 #if HAVE_GTK
00060 #include <gio/gio.h>
00061 #include <gtk/gtk.h>
00062 #include "interface.h"
00063 #endif
00064
00065 #define DEBUG 0
00066
00076 #if HAVE_GTK
00077 #define ERROR_TYPE GTK_MESSAGE_ERROR
00078 #define INFO_TYPE GTK_MESSAGE_INFO
00079 #else
00080 #define ERROR_TYPE 0
00081 #define INFO_TYPE 0
00082 #endif
00083 #ifdef G_OS_WIN32
00084 #define INPUT_FILE "test-ga-win.xml"
00085 #define RM "del"
00086 #else
00087 #define INPUT_FILE "test-ga.xml" 00088 #define RM "rm"
00089 #endif
00090
00091 int ntasks;
00092 unsigned int nthreads;
00093 unsigned int nthreads_gradient;
00095 GMutex mutex[1];
00096 void (*calibrate_algorithm) ();
00098 double (*calibrate_estimate_gradient) (unsigned int variable,
                                               unsigned int estimate);
00101 Input input[1];
00103 Calibrate calibrate[1];
00104
00105 const xmlChar *result_name = (xmlChar *) "result";
00107 const xmlChar *variables_name = (xmlChar *) "variables";
00110 const xmlChar *template[MAX_NINPUTS] = {
00111
        XML_TEMPLATE1, XML_TEMPLATE2, XML_TEMPLATE3,
     XML TEMPLATE4.
00112 XML_TEMPLATE5, XML_TEMPLATE6, XML_TEMPLATE7,
      XML_TEMPLATE8
00113 };
00114
00116
00120 };
00122 const double precision[NPRECISIONS] = {
00123 1., 0.1, 0.01, 1e-3, 1e-4, 1e-5, 1e-6, 1e-7, 1e-8, 1e-9, 1e-10, 1e-11, 1e-12, 00124 1e-13, 1e-14
00125 };
00126
00127 const char *logo[] = {
      "32 32 3 1",
" c None",
00128
00129
              c #0000FF",
00130
        "+
              c #FF0000".
00131
00132
00133
00134
00135
00136
00137
00138
00139
                            +++
00140
                           +++++
00141
                           +++++
00142
                           +++++
00143
             +++
                            +++
                                    +++
            +++++
                                   +++++
00144
            +++++
00145
                                   ++++
             +++++
                                   ++++
00146
00147
             +++
00148
00149
                    +++
00150
                    +++++
00151
                    +++++
```

```
00153
                     +++
00154
00155
00156
00157
00158
00159
00160
00161
00162
00163
00164 };
00165
00166 /*
00167 const char * logo[] = { 00168 "32 32 3 1",
00169 " c #FFFFFFFFFF,
            c #00000000FFFF",
00171 "X
00172 "
           c #FFFF00000000",
00173 "
00174 "
00175 "
00176 "
00177 "
00178 "
00179 "
                          XXX
00180 "
                          XXXXX
00181 "
                          XXXXX
00182 "
                          XXXXX
00183 "
00184 "
           XXX
                           XXX
                                  XXX
          XXXXX
                                 XXXXX
                           .
00185 "
          XXXXX
                                 XXXXX
00186 "
          XXXXX
                                 XXXXX
00187 "
           XXX
                                  XXX
00188 "
00189 "
                   XXX
00190 "
                  XXXXX
00191 "
                  XXXXX
00192 "
                  XXXXX
00193 "
                   XXX
00194 "
                    .
00195 "
00196 "
00197 "
00198 "
00199 "
00200 "
00201 "
00202 "
00203 "
00204 */
00205
00206 #if HAVE_GTK
00207 Options options[1];
00209 Running running[1];
00211 Window window[1];
00213 #endif
00214
00225 void
00226 show_message (char *title, char *msg, int type)
00227 {
00228 #if HAVE_GTK
00229
        GtkMessageDialog *dlg;
00230
00231
        // Creating the dialog
00232
        dlg = (GtkMessageDialog *) gtk_message_dialog_new
00233
           (window->window, GTK_DIALOG_MODAL, type, GTK_BUTTONS_OK, "%s", msg);
00234
00235
        // Setting the dialog title
00236
        gtk_window_set_title (GTK_WINDOW (dlg), title);
00237
        // Showing the dialog and waiting response
gtk_dialog_run (GTK_DIALOG (dlg));
00238
00239
00240
00241
         // Closing and freeing memory
00242
        gtk_widget_destroy (GTK_WIDGET (dlg));
00243
00244 #else
00245 printf ("%s: %s\n", title, msg);
00246 #endif
00247 }
00248
00255 void
00256 show_error (char *msg)
00257 {
```

```
show_message (gettext ("ERROR!"), msg, ERROR_TYPE);
00259 }
00260
00273 int.
00274 xml_node_get_int (xmlNode * node, const xmlChar * prop, int *error_code)
00275 {
00277
        xmlChar *buffer;
00278
        buffer = xmlGetProp (node, prop);
00279
        if (!buffer)
00280
         *error_code = 1;
00281
        else
00282
        {
         if (sscanf ((char *) buffer, "%d", &i) != 1)
00283
00284
             *error_code = 2;
00285
          else
             *error_code = 0;
00286
00287
           xmlFree (buffer);
00288
00289
       return i;
00290 }
00291
00304 unsigned int
00305 xml_node_get_uint (xmlNode * node, const xmlChar * prop, int *error_code)
00306 {
00307
       unsigned int i = 0;
00308
        xmlChar *buffer;
00309
       buffer = xmlGetProp (node, prop);
00310
       if (!buffer)
00311
         *error_code = 1;
00312
       else
00313
        {
00314
          if (sscanf ((char *) buffer, "%u", &i) != 1)
00315
              *error_code = 2;
00316
            else
             *error_code = 0;
00317
00318
           xmlFree (buffer);
00319
00320
       return i;
00321 }
00322
00335 double
00336 xml_node_get_float (xmlNode * node, const xmlChar * prop, int *error_code)
00337 {
00338
      double x = 0.;
00339
        xmlChar *buffer;
00340
       buffer = xmlGetProp (node, prop);
00341
        if (!buffer)
00342
         *error_code = 1;
00343
        else
00344
        {
00345
          if (sscanf ((char *) buffer, "%lf", &x) != 1)
00346
              *error_code = 2;
00347
           else
00348
             *error_code = 0;
00349
           xmlFree (buffer);
00350
00351
       return x;
00352 }
00353
00364 void
00365 xml_node_set_int (xmlNode * node, const xmlChar * prop, int value)
00366 {
00367 xmlChar buffer[64];
00368 snprintf ((char *) buffer, 64, "%d", value);
00369
       xmlSetProp (node, prop, buffer);
00370 }
00371
00383 void
00384 xml_node_set_uint (xmlNode * node, const xmlChar * prop, unsigned int value)
00385 {
00386
       xmlChar buffer[64];
       snprintf ((char *) buffer, 64, "%u", value);
00387
00388
        xmlSetProp (node, prop, buffer);
00389 }
00390
00402 void
00403 xml_node_set_float (xmlNode * node, const xmlChar * prop, double value)
00404 {
00405 xmlChar buffer[64];
00406 snprintf ((char *) buffer, 64, "%.141g", value);
       xmlSetProp (node, prop, buffer);
00408 }
00409
00414 void
00415 input_new ()
00416 {
```

```
unsigned int i;
00418 #if DEBUG
        fprintf (stderr, "input_new: start\n");
00419
00420 #endif
00421 input->nvariables = input->nexperiments = input->ninputs = input->
     nsteps = 0:
00422 input->simulator = input->evaluator = input->directory = input->
     name
        = input->result = input->variables = NULL;
input->experiment = input->label = NULL;
00423
00424
        input->recision = input->nsweeps = input->nbits = NULL;
input->rangemin = input->rangemax = input->rangeminabs = input->
00425
00426
     rangemaxabs
00427
          = input->weight = input->step = NULL;
00428
        for (i = 0; i < MAX_NINPUTS; ++i)</pre>
00429 input->template[i] = NULL;
00430 #if DEBUG
00431
       fprintf (stderr, "input_new: end\n");
00432 #endif
00433 }
00434
00439 void
00440 input_free ()
00441 {
00442
        unsigned int i, j;
00444
        fprintf (stderr, "input_free: start\n");
00445 #endif
00446
        g_free (input->name);
00447
        g_free (input->directory);
00448
        for (i = 0; i < input->nexperiments; ++i)
00449
00450
            xmlFree (input->experiment[i]);
00451
            for (j = 0; j < input->ninputs; ++j)
00452
              xmlFree (input->template[j][i]);
00453
            g_free (input->template[j]);
00454
00455
        g_free (input->experiment);
00456
        for (i = 0; i < input->ninputs; ++i)
00457
          g_free (input->template[i]);
00458
        for (i = 0; i < input->nvariables; ++i)
00459
         xmlFree (input->label[i]);
00460
        g free (input->label);
        g_free (input->precision);
00461
        g_free (input->rangemin);
00462
        g_free (input->rangemax);
00463
00464
        g_free (input->rangeminabs);
00465
        g_free (input->rangemaxabs);
        g_free (input->weight);
00466
        g_free (input->step);
00467
00468
        g_free (input->nsweeps);
00469
        g_free (input->nbits);
00470
        xmlFree (input->evaluator);
00471
        xmlFree (input->simulator);
00472
        xmlFree (input->result);
        xmlFree (input->variables);
00473
      input->nexperiments = input->ninputs = input->nvariables = input->
      nsteps = 0;
00475 #if DEBUG
       fprintf (stderr, "input_free: end\n");
00476
00477 #endif
00478 }
00479
00487 int
00488 input_open (char *filename)
00489 {
00490
        char buffer2[64];
        char *buffert[MAX_NINPUTS] =
00491
         { NULL, NULL, NULL, NULL, NULL, NULL, NULL, NULL };
00492
00493
        xmlDoc *doc;
00494
        xmlNode *node, *child;
00495
        xmlChar *buffer;
00496
        char *msg;
00497
        int error_code;
00498
        unsigned int i;
00499
00500 #if DEBUG
00501
       fprintf (stderr, "input_open: start\n");
00502 #endif
00503
00504
        // Resetting input data
00505
        buffer = NULL;
00506
        input_new ();
00507
00508
        // Parsing the input file
00509 #if DEBUG
00510
        fprintf (stderr, "input open: parsing the input file %s\n", filename);
```

```
00511 #endif
      doc = xmlParseFile (filename);
00512
00513
        if (!doc)
00514
         {
00515
           msg = gettext ("Unable to parse the input file");
00516
            goto exit on error;
00517
00518
00519
        // Getting the root node
00520 #if DEBUG
00521
        fprintf (stderr, "input_open: getting the root node\n");
00522 #endif
00523
        node = xmlDocGetRootElement (doc);
00524
        if (xmlStrcmp (node->name, XML_CALIBRATE))
00525
00526
            msg = gettext ("Bad root XML node");
00527
            goto exit_on_error;
          }
00528
00529
00530
        // Getting results file names
00531
        input->result = (char *) xmlGetProp (node, XML_RESULT);
00532
           (!input->result)
        input->result = (char *) xmlStrdup (result_name);
input->variables = (char *) xmlGetProp (node, XML_VARIABLES);
00533
00534
00535
        if (!input->variables)
00536
         input->variables = (char *) xmlStrdup (variables_name);
00537
00538
        // Opening simulator program name
        input->simulator = (char *) xmlGetProp (node, XML_SIMULATOR);
if (!input->simulator)
00539
00540
00541
         {
00542
            msg = gettext ("Bad simulator program");
00543
            goto exit_on_error;
00544
00545
        // Opening evaluator program name
00546
        input->evaluator = (char *) xmlGetProp (node, XML_EVALUATOR);
00547
00548
00549
        // Obtaining pseudo-random numbers generator seed
        if (!xmlHasProp (node, XML_SEED))
  input->seed = DEFAULT_RANDOM_SEED;
00550
00551
00552
        else
00553
         {
00554
            input->seed = xml_node_get_uint (node, XML_SEED, &error_code);
00555
            if (error_code)
00556
00557
                msg = gettext ("Bad pseudo-random numbers generator seed");
00558
                goto exit_on_error;
              }
00559
00560
         }
00561
00562
         // Opening algorithm
00563
        buffer = xmlGetProp (node, XML_ALGORITHM);
00564
        if (!xmlStrcmp (buffer, XML_MONTE_CARLO))
00565
00566
            input->algorithm = ALGORITHM MONTE CARLO;
00567
00568
             // Obtaining simulations number
00569
            input->nsimulations
00570
              = xml_node_get_int (node, XML_NSIMULATIONS, &error_code);
00571
             if (error_code)
00572
              {
00573
                msg = gettext ("Bad simulations number");
00574
                goto exit_on_error;
00575
00576
        else if (!xmlStrcmp (buffer, XML_SWEEP))
00577
          input->algorithm = ALGORITHM_SWEEP;
00578
00579
        else if (!xmlStrcmp (buffer, XML_GENETIC))
00580
00581
             input->algorithm = ALGORITHM_GENETIC;
00582
00583
             // Obtaining population
            if (xmlHasProp (node, XML_NPOPULATION))
00584
00585
              {
00586
                 input->nsimulations
00587
                    xml_node_get_uint (node, XML_NPOPULATION, &error_code);
00588
                 if (error_code || input->nsimulations < 3)</pre>
00589
00590
                    msg = gettext ("Invalid population number");
00591
                     goto exit_on_error;
00592
                  }
00593
00594
            else
00595
              {
                msg = gettext ("No population number");
00596
00597
                 goto exit on error;
```

```
00598
               }
00599
00600
             // Obtaining generations
             if (xmlHasProp (node, XML_NGENERATIONS))
00601
00602
00603
                 input->niterations
                    = xml_node_get_uint (node, XML_NGENERATIONS, &error_code);
00604
00605
                  if (error_code || !input->niterations)
00606
00607
                     msg = gettext ("Invalid generations number");
00608
                     goto exit_on_error;
00609
00610
               }
00611
             else
00612
               {
00613
                 msg = gettext ("No generations number");
00614
                 goto exit_on_error;
00615
00616
00617
             // Obtaining mutation probability
00618
             if (xmlHasProp (node, XML_MUTATION))
00619
00620
                 input->mutation_ratio
                 = xml_node_get_float (node, XML_MUTATION, &error_code);
if (error_code || input->mutation_ratio < 0.</pre>
00621
00622
                     || input->mutation_ratio >= 1.)
00623
00624
00625
                     msg = gettext ("Invalid mutation probability");
00626
                      goto exit_on_error;
00627
00628
00629
             else
00630
00631
                 msg = gettext ("No mutation probability");
00632
                 goto exit_on_error;
00633
00634
00635
             // Obtaining reproduction probability
00636
             if (xmlHasProp (node, XML_REPRODUCTION))
00637
00638
                 input->reproduction_ratio
                 = xml_node_get_float (node, XML_REPRODUCTION, &error_code);
if (error_code || input->reproduction_ratio < 0.</pre>
00639
00640
00641
                      || input->reproduction_ratio >= 1.0)
00642
00643
                      msg = gettext ("Invalid reproduction probability");
00644
                      goto exit_on_error;
00645
00646
               }
00647
             else
00648
               {
00649
                 msg = gettext ("No reproduction probability");
00650
                 goto exit_on_error;
00651
00652
00653
             // Obtaining adaptation probability
             if (xmlHasProp (node, XML_ADAPTATION))
00655
               {
                 input->adaptation_ratio
00656
                 = xml_node_get_float (node, XML_ADAPTATION, &error_code);
if (error_code || input->adaptation_ratio < 0.</pre>
00657
00658
00659
                      || input->adaptation_ratio >= 1.)
00660
                   {
00661
                     msg = gettext ("Invalid adaptation probability");
00662
                     goto exit_on_error;
                   }
00663
00664
               }
00665
             else
00666
              {
                 msg = gettext ("No adaptation probability");
00668
                 goto exit_on_error;
00669
00670
00671
             // Checking survivals
00672
             i = input->mutation_ratio * input->nsimulations;
00673
             i += input->reproduction_ratio * input->nsimulations;
00674
             i += input->adaptation_ratio * input->nsimulations;
00675
             if (i > input->nsimulations - 2)
00676
               {
00677
                 msg = gettext
00678
                   ("No enough survival entities to reproduce the population");
00679
                 goto exit_on_error;
00680
00681
          }
00682
        else
00683
00684
             msg = gettext ("Unknown algorithm");
```

```
goto exit_on_error;
00686
00687
        xmlFree (buffer);
00688
        buffer = NULL;
00689
00690
        if (input->algorithm == ALGORITHM_MONTE_CARLO
            || input->algorithm == ALGORITHM_SWEEP)
00692
00693
00694
             // Obtaining iterations number
00695
            input->niterations
00696
              = xml node get uint (node, XML NITERATIONS, &error code);
            if (error_code == 1)
00697
              input->niterations = 1;
00698
00699
            else if (error_code)
00700
             {
                msg = gettext ("Bad iterations number");
00701
00702
                goto exit_on_error;
00703
00704
00705
             // Obtaining best number
00706
             if (xmlHasProp (node, XML_NBEST))
00707
              {
                input->nbest = xml_node_get_uint (node,
00708
     XML_NBEST, &error_code);
00709
                if (error_code || !input->nbest)
00710
00711
                    msg = gettext ("Invalid best number");
00712
                     goto exit_on_error;
00713
                  }
00714
              }
00715
            else
00716
              input->nbest = 1;
00717
00718
             // Obtaining tolerance
            if (xmlHasProp (node, XML_TOLERANCE))
00719
00720
              {
00721
                 input->tolerance
00722
                   = xml_node_get_float (node, XML_TOLERANCE, &error_code);
00723
                 if (error_code || input->tolerance < 0.)</pre>
00724
00725
                    msg = gettext ("Invalid tolerance");
00726
                     goto exit_on_error;
00727
                   }
00728
00729
             else
00730
              input->tolerance = 0.;
00731
00732
             // Getting gradient method parameters
00733
            if (xmlHasProp (node, XML_NSTEPS))
00734
              {
                input->nsteps = xml_node_get_uint (node,
00735
     XML_NSTEPS, &error_code);
00736
                if (error_code || !input->nsteps)
00737
                  {
00738
                     msg = gettext ("Invalid steps number");
00739
                     goto exit_on_error;
00740
00741
                 buffer = xmlGetProp (node, XML_GRADIENT_METHOD);
                if (!xmlStrcmp (buffer, XML_COORDINATES))
  input->gradient_method = GRADIENT_METHOD_COORDINATES;
00742
00743
00744
                 else if (!xmlStrcmp (buffer, XML_RANDOM))
00745
                  {
00746
                     input->gradient_method = GRADIENT_METHOD_RANDOM;
00747
                     input->nestimates
00748
                       = xml_node_get_uint (node, XML_NESTIMATES, &error_code);
00749
                     if (error_code || !input->nestimates)
00750
00751
                        msq = gettext ("Invalid estimates number");
00752
                         goto exit_on_error;
00753
00754
00755
                 else
00756
                  {
00757
                     msg = gettext ("Unknown method to estimate the gradient");
00758
                     goto exit_on_error;
00759
00760
                 xmlFree (buffer);
00761
                 buffer = NULL:
00762
                 if (xmlHasProp (node, XML_RELAXATION))
00763
00764
                     input->relaxation
                     = xml_node_get_float (node, XML_RELAXATION, &error_code);
if (error_code || input->relaxation < 0.</pre>
00765
00766
00767
                         || input->relaxation > 2.)
00768
00769
                         msg = gettext ("Invalid relaxation parameter");
```

```
goto exit_on_error;
00771
00772
00773
               else
00774
                 input->relaxation = DEFAULT RELAXATION;
00775
             }
00776
            else
00777
             input->nsteps = 0;
00778
         }
00779
00780
       // Reading the experimental data
00781
       for (child = node->children; child; child = child->next)
00782
00783
            if (xmlStrcmp (child->name, XML_EXPERIMENT))
00784
             break;
00785 #if DEBUG
           fprintf (stderr, "input_open: nexperiments=%u\n", input->nexperiments);
00786
00787 #endif
           if (xmlHasProp (child, XML_NAME))
00789
             buffer = xmlGetProp (child, XML_NAME);
00790
            else
00791
             {
               00792
00793
00794
                         input->nexperiments + 1, gettext ("no data file name"));
00795
               msg = buffer2;
00796
               goto exit_on_error;
00797
00798 #if DEBUG
           fprintf (stderr, "input_open: experiment=%s\n", buffer);
00799
00800 #endif
00801
           input->weight = g_realloc (input->weight,
00802
                                       (1 + input->nexperiments) * sizeof (double));
00803
           if (xmlHasProp (child, XML_WEIGHT))
00804
               input->weight[input->nexperiments]
00805
                  = xml_node_get_float (child, XML_WEIGHT, &error_code);
00806
                if (error_code)
00808
                 {
00809
                    snprintf (buffer2, 64, "%s %s: %s",
00810
                             gettext ("Experiment"), buffer, gettext ("bad weight"));
                   msq = buffer2;
00811
00812
                   goto exit_on_error;
00813
                 }
00814
00815
            else
00816
             input->weight[input->nexperiments] = 1.;
00817 #if DEBUG
           00818
00819
00820 #endif
00821
           if (!input->nexperiments)
00822
             input->ninputs = 0;
00823 #if DEBUG
           fprintf (stderr, "input_open: template[0]\n");
00824
00825 #endif
           if
              (xmlHasProp (child, XML_TEMPLATE1))
00827
             {
00828
               input->template[0]
00829
                  = (char **) g_realloc (input->template[0],
                                         (1 + input->nexperiments) * sizeof (char *));
00830
00831
               buffert[0] = (char *) xmlGetProp (child, template[0]);
00832 #if DEBUG
              fprintf (stderr, "input_open: experiment=%u template1=%s\n",
00833
00834
                        input->nexperiments, buffert[0]);
00835 #endif
               if (!input->nexperiments)
00836
00837
                 ++input->ninputs;
00838 #if DEBUG
               fprintf (stderr, "input_open: ninputs=%u\n", input->ninputs);
00840 #endif
00841
             }
00842
           else
00843
             {
00844
               snprintf (buffer2, 64, "%s %s: %s",
                         gettext ("Experiment"), buffer, gettext ("no template"));
00845
00846
               msg = buffer2;
00847
               goto exit_on_error;
00848
00849
           for (i = 1; i < MAX NINPUTS; ++i)</pre>
00850
00851 #if DEBUG
00852
               fprintf (stderr, "input_open: template%u\n", i + 1);
00853 #endif
00854
               if (xmlHasProp (child, template[i]))
00855
00856
                   if (input->nexperiments && input->ninputs <= i)</pre>
```

```
00858
                         snprintf (buffer2, 64, "%s %s: %s",
                                   gettext ("Experiment"),
00859
                                   buffer, gettext ("bad templates number"));
00860
                         msg = buffer2;
00861
00862
                        while (i-- > 0)
                          xmlFree (buffert[i]);
00864
                        goto exit_on_error;
00865
00866
                    input->template[i] = (char **)
                      00867
00868
00869
                    buffert[i] = (char *) xmlGetProp (child, template[i]);
00870 #if DEBUG
00871
                    fprintf (stderr, "input_open: experiment=%u template%u=%s\n",
00872
                              input->nexperiments, i + 1,
00873
                              input->template[i][input->nexperiments]);
00874 #endif
                    if (!input->nexperiments)
00876
                      ++input->ninputs;
00877 #if DEBUG
00878
                    fprintf (stderr, "input_open: ninputs=%u\n", input->ninputs);
00879 #endif
00880
00881
                else if (input->nexperiments && input->ninputs >= i)
00883
                    snprintf (buffer2, 64, "%s %s: %s%u",
00884
                               gettext ("Experiment"),
                               buffer, gettext ("no template"), i + 1);
00885
                    msg = buffer2;
00886
00887
                    while (i-- > 0)
00888
                      xmlFree (buffert[i]);
00889
                    goto exit_on_error;
00890
00891
                else
00892
                  break;
              }
00893
            input->experiment
00895
              = g_realloc (input->experiment,
00896
                            (1 + input->nexperiments) * sizeof (char *));
00897
            input->experiment[input->nexperiments] = (char *) buffer;
00898
            for (i = 0; i < input->ninputs; ++i)
              input->template[i][input->nexperiments] = buffert[i];
00899
00900
            ++input->nexperiments;
00901 #if DEBUG
00902
            fprintf (stderr, "input_open: nexperiments=%u\n", input->nexperiments);
00903 #endif
00904
        if (!input->nexperiments)
00905
00906
         {
00907
            msg = gettext ("No calibration experiments");
00908
           goto exit_on_error;
00909
00910
        buffer = NULL:
00911
00912
        // Reading the variables data
00913
        for (; child; child = child->next)
00914
00915
            if (xmlStrcmp (child->name, XML_VARIABLE))
00916
                snprintf (buffer2, 64, "%s %u: %s",
00917
                          gettext ("Variable"),
00918
00919
                           input->nvariables + 1, gettext ("bad XML node"));
00920
                msg = buffer2;
00921
                goto exit_on_error;
00922
            if (xmlHasProp (child, XML_NAME))
buffer = xmlGetProp (child, XML_NAME);
00923
00924
00925
            else
00926
             {
00927
                snprintf (buffer2, 64, "%s %u: %s",
00928
                          gettext ("Variable"),
00929
                          input->nvariables + 1, gettext ("no name"));
                msg = buffer2:
00930
00931
                goto exit on error;
00932
00933
            if (xmlHasProp (child, XML_MINIMUM))
00934
00935
                input->rangemin = g_realloc
00936
                (input->rangemin, (1 + input->nvariables) * sizeof (double));
input->rangeminabs = g_realloc
00937
                (input->rangeminabs, (1 + input->nvariables) * sizeof (double));
input->rangemin[input->nvariables]
00938
00939
00940
                   = xml_node_get_float (child, XML_MINIMUM, &error_code);
00941
                 if (error_code)
00942
00943
                    snprintf (buffer2, 64, "%s %s: %s",
```

```
gettext ("Variable"), buffer, gettext ("bad minimum"));
00945
                   msg = buffer2;
00946
                   goto exit_on_error;
00947
               if (xmlHasProp (child, XML_ABSOLUTE_MINIMUM))
00948
00949
                   input->rangeminabs[input->nvariables]
00951
                       xml_node_get_float (child,
     XML_ABSOLUTE_MINIMUM, &error_code);
00952
                   if (error_code)
00953
                       00954
00955
00956
                                 buffer, gettext ("bad absolute minimum"));
00957
                       msg = buffer2;
00958
                       goto exit_on_error;
00959
00960
                 }
00961
               else
00962
                 input->rangeminabs[input->nvariables] = -G_MAXDOUBLE;
00963
                if (input->rangemin[input->nvariables]
00964
                   < input->rangeminabs[input->nvariables])
00965
                   00966
00967
00968
                             buffer, gettext ("minimum range not allowed"));
00969
                   msg = buffer2;
00970
                   goto exit_on_error;
                 }
00971
00972
             }
00973
           else
00974
             {
00975
               snprintf (buffer2, 64, "%s %s: %s",
00976
                         gettext ("Variable"), buffer, gettext ("no minimum range"));
00977
               msq = buffer2;
00978
               goto exit_on_error;
00979
00980
           if (xmlHasProp (child, XML_MAXIMUM))
00981
             {
00982
               input->rangemax = g_realloc
               (input->rangemax, (1 + input->nvariables) * sizeof (double));
input->rangemaxabs = g_realloc
00983
00984
               (input->rangemaxabs, (1 + input->nvariables) * sizeof (double));
input->rangemax[input->nvariables]
00985
00986
                  = xml_node_get_float (child, XML_MAXIMUM, &error_code);
00987
00988
               if (error_code)
00989
                   00990
00991
                   msq = buffer2;
00992
00993
                   goto exit_on_error;
00994
00995
               if (xmlHasProp (child, XML_ABSOLUTE_MAXIMUM))
00996
                   input->rangemaxabs[input->nvariables]
00997
                     = xml_node_get_float (child,
00998
     XML_ABSOLUTE_MAXIMUM, &error_code);
00999
                   if (error_code)
01000
                       01001
01002
                                 buffer, gettext ("bad absolute maximum"));
01003
01004
                       msg = buffer2;
01005
                       goto exit_on_error;
01006
01007
01008
               else
01009
                 input->rangemaxabs[input->nvariables] = G MAXDOUBLE;
               if (input->rangemax[input->nvariables]
01010
                   > input->rangemaxabs[input->nvariables])
01012
01013
                   snprintf (buffer2, 64, "%s %s: %s",
                             gettext ("Variable"),
01014
                             buffer, gettext ("maximum range not allowed"));
01015
01016
                   msq = buffer2;
01017
                   goto exit_on_error;
01018
                 }
01019
01020
           else
01021
             {
               snprintf (buffer2, 64, "%s %s: %s",
01022
                         gettext ("Variable"), buffer, gettext ("no maximum range"));
01024
               msg = buffer2;
01025
               goto exit_on_error;
01026
           if (input->rangemax[input->nvariables]
01027
01028
                < input->rangemin[input->nvariables])
```

```
{
01030
              snprintf (buffer2, 64, "%s %s: %s",
01031
                        gettext ("Variable"), buffer, gettext ("bad range"));
               msa = buffer2;
01032
01033
              goto exit_on_error;
01034
           input->precision = g_realloc
01036
             (input->precision, (1 + input->nvariables) * sizeof (unsigned int));
           if (xmlHasProp (child, XML_PRECISION))
01037
01038
               input->precision[input->nvariables]
01039
                 = xml_node_get_uint (child, XML_PRECISION, &error_code);
01040
               if (error_code || input->precision[input->nvariables] >=
01041
     NPRECISIONS)
01042
                   01043
01044
                            buffer, gettext ("bad precision"));
01045
                  msg = buffer2;
01046
01047
                  goto exit_on_error;
01048
01049
             }
           else
01050
            input->precision[input->nvariables] =
01051
     DEFAULT_PRECISION;
01052
           if (input->algorithm == ALGORITHM_SWEEP)
01053
01054
               if (xmlHasProp (child, XML_NSWEEPS))
01055
01056
                  input->nsweeps = (unsigned int *)
01057
                    g_realloc (input->nsweeps,
01058
                               (1 + input->nvariables) * sizeof (unsigned int));
01059
                   input->nsweeps[input->nvariables]
                     = xml_node_get_uint (child, XML_NSWEEPS, &error_code);
01060
01061
                   if (error_code || !input->nsweeps[input->nvariables])
01062
                      01063
01064
01065
                                buffer, gettext ("bad sweeps"));
01066
                      msg = buffer2;
01067
                      goto exit_on_error;
                    }
01068
01069
                 }
01070
               else
01071
                {
                   snprintf (buffer2, 64, "%s %s: %s",
01072
01073
                            gettext ("Variable"),
01074
                            buffer, gettext ("no sweeps number"));
01075
                  msg = buffer2;
01076
                  goto exit_on_error;
01078 #if DEBUG
         fprintf (stderr, "input_open: nsweeps=%u nsimulations=%u\n",
01079
01080
                       input->nsweeps[input->nvariables], input->
     nsimulations);
01081 #endif
01082
01083
           if (input->algorithm == ALGORITHM_GENETIC)
01084
               \//\ Obtaining bits representing each variable
01085
               if (xmlHasProp (child, XML_NBITS))
01086
01087
01088
                  input->nbits = (unsigned int *)
                    g_realloc (input->nbits,
01089
01090
                               (1 + input->nvariables) * sizeof (unsigned int));
01091
                   i = xml_node_get_uint (child, XML_NBITS, &error_code);
01092
                   if (error_code || !i)
01093
                    {
                      01094
01095
01096
                                buffer, gettext ("invalid bits number"));
                       msg = buffer2;
01097
01098
                      goto exit_on_error;
01099
01100
                   input->nbits[input->nvariables] = i;
01101
01102
01103
                  01104
01105
                            buffer, gettext ("no bits number"));
01106
01107
                  msg = buffer2;
01108
                  goto exit_on_error;
01109
01110
           else if (input->nsteps)
01111
01112
```

```
input->step = (double *)
                 g_realloc (input->step, (1 + input->nvariables) * sizeof (double));
01114
01115
                input->step[input->nvariables]
                 = xml_node_get_float (child, XML_STEP, &error_code);
01116
01117
                if (error_code || input->step[input->nvariables] < 0.)</pre>
01118
                 {
                   01119
01120
01121
                              buffer, gettext ("bad step size"));
01122
                   msg = buffer2;
01123
                   goto exit_on_error;
01124
01125
01126
            input->label = g_realloc
01127
              (input->label, (1 + input->nvariables) * sizeof (char *));
01128
            input->label[input->nvariables] = (char *) buffer;
01129
            ++input->nvariables:
01130
01131
       if (!input->nvariables)
01132
        {
01133
           msg = gettext ("No calibration variables");
01134
           goto exit_on_error;
01135
01136
       buffer = NULL:
01137
01138
       // Getting the working directory
01139
       input->directory = g_path_get_dirname (filename);
01140
       input->name = g_path_get_basename (filename);
01141
       // Closing the XML document
01142
01143
       xmlFreeDoc (doc);
01144
01145 #if DEBUG
01146 fprintf (stderr, "input_open: end\n");
01147 #endif
01148
       return 1;
01149
01150 exit_on_error:
01151 xmlFree (buffer);
01152 xmlFreeDoc (doc);
01153 show_error (msq);
       show_error (msg);
01154
       input_free ();
01155 #if DEBUG
01156
       fprintf (stderr, "input_open: end\n");
01157 #endif
01158
       return 0;
01159 }
01160
01172 void
01173 calibrate_input (unsigned int simulation, char *input, GMappedFile * template)
01174 {
01175
       unsigned int i;
01176
       char buffer[32], value[32], *buffer2, *buffer3, *content;
01177
       FILE *file;
01178
       gsize length;
01179
       GRegex *regex;
01180
01181 #if DEBUG
01182 fprintf (stderr, "calibrate_input: start\n");
01183 #endif
01184
01185
       // Checking the file
01186
       if (!template)
        goto calibrate_input_end;
01187
01188
01189
       // Opening template
       content = g_mapped_file_get_contents (template);
01190
01191
       length = g_mapped_file_get_length (template);
01192 #if DEBUG
01193 fprintf (stderr, "calibrate_input: length=%lu\ncontent:\n%s", length,
01194
                content);
01195 #endif
01196 file = g_fopen (input, "w");
01197
01198
       // Parsing template
01199
       for (i = 0; i < calibrate->nvariables; ++i)
01200
01201 #if DEBUG
           fprintf (stderr, "calibrate_input: variable=%u\n", i);
01202
01203 #endif
          snprintf (buffer, 32, "@variable%u@", i + 1);
01204
           regex = g_regex_new (buffer, 0, 0, NULL);
01206
01207
01208
               buffer2 = g_regex_replace_literal (regex, content, length, 0,
01209
                                                   calibrate->label[i], 0, NULL);
01210 #if DEBUG
```

```
fprintf (stderr, "calibrate_input: buffer2\n%s", buffer2);
01212 #endif
01213
01214
            else
01215
              {
                length = strlen (buffer3);
01216
                buffer2 = g_regex_replace_literal (regex, buffer3, length, 0,
01217
01218
                                                      calibrate->label[i], 0, NULL);
01219
                g_free (buffer3);
01220
01221
            q_regex_unref (regex);
01222
            length = strlen (buffer2);
snprintf (buffer, 32, "@value%u@", i + 1);
01223
01224
            regex = g_regex_new (buffer, 0, 0, NULL);
            snprintf (value, 32, format[calibrate->precision[i]],
01225
01226
                       calibrate->value[simulation * calibrate->nvariables + i]);
01227
01228 #if DEBUG
            fprintf (stderr, "calibrate_input: value=%s\n", value);
01230 #endif
01231
            buffer3 = g_regex_replace_literal (regex, buffer2, length, 0, value,
01232
                                                  0, NULL);
01233
            g_free (buffer2);
01234
            g_regex_unref (regex);
01235
01236
01237
        // Saving input file
01238
       fwrite (buffer3, strlen (buffer3), sizeof (char), file);
        g_free (buffer3);
01239
01240
        fclose (file):
01241
01242 calibrate_input_end:
01243 #if DEBUG
01244
        fprintf (stderr, "calibrate_input: end\n");
01245 #endif
01246
        return;
01247 }
01248
01259 double
01260 calibrate_parse (unsigned int simulation, unsigned int experiment)
01261 {
01262
        unsigned int i;
01263
        double e:
01264
       char buffer[512], input[MAX_NINPUTS][32], output[32], result[32], *buffer2,
01265
          *buffer3, *buffer4;
01266
       FILE *file_result;
01267
01268 #if DEBUG
       fprintf (stderr, "calibrate_parse: start\n");
fprintf (stderr, "calibrate_parse: simulation=%u experiment=%u\n", simulation,
01269
01270
01271
                 experiment);
01272 #endif
01273
01274
        // Opening input files
01275
        for (i = 0; i < calibrate->ninputs; ++i)
01276
             snprintf (&input[i][0], 32, "input-%u-%u-%u", i, simulation, experiment);
01277
01278 #if DEBUG
01279
            fprintf (stderr, "calibrate_parse: i=%u input=%s\n", i, &input[i][0]);
01280 #endif
            01281
01282
01283
        for (; i < MAX_NINPUTS; ++i)</pre>
01284
01285
          strcpy (&input[i][0], "");
01286 #if DEBUG
        fprintf (stderr, "calibrate_parse: parsing end\n");
01287
01288 #endif
01289
        // Performing the simulation
01291
        snprintf (output, 32, "output-%u-%u", simulation, experiment);
01292
        buffer2 = g_path_get_dirname (calibrate->simulator);
        buffer3 = g_path_get_basename (calibrate->simulator);
01293
        buffer4 = g_build_filename (buffer2, buffer3, NULL);
snprintf (buffer, 512, "\"%s\" %s %s %s %s %s %s %s %s %s",
    buffer4, input[0], input[1], input[2], input[3], input[4], input[5],
01294
01295
01296
01297
                  input[6], input[7], output);
01298
       g_free (buffer4);
01299
        g_free (buffer3);
01300
        g_free (buffer2);
01301 #if DEBUG
01302
        fprintf (stderr, "calibrate_parse: %s\n", buffer);
01303 #endif
01304
        system (buffer);
01305
        // Checking the objective value function
01306
01307
        if (calibrate->evaluator)
```

```
01308
01309
            snprintf (result, 32, "result-%u-%u", simulation, experiment);
01310
            buffer2 = g_path_get_dirname (calibrate->evaluator);
            buffer3 = g_path_get_basename (calibrate->evaluator);
01311
            buffer4 = g_build_filename (buffer2, buffer3, NULL); snprintf (buffer, 512, "\"%s\" %s %s %s",
01312
01313
                       buffer4, output, calibrate->experiment[experiment], result);
01314
01315
            g_free (buffer4);
            g_free (buffer3);
01316
01317
            g_free (buffer2);
01318 #if DEBUG
            fprintf (stderr, "calibrate_parse: %s\n", buffer);
01319
01320 #endif
01321
            system (buffer);
01322
            file_result = g_fopen (result, "r");
            e = atof (fgets (buffer, 512, file_result));
fclose (file_result);
01323
01324
01325
          }
01326
        else
01327
        {
01328
            strcpy (result, "");
            file_result = g_fopen (output, "r");
01329
            e = atof (fgets (buffer, 512, file_result));
01330
01331
            fclose (file_result);
01332
          }
01333
        // Removing files
01334
01335 #if !DEBUG
       for (i = 0; i < calibrate->ninputs; ++i)
01336
01337
01338
            if (calibrate->file[i][0])
01339
              {
01340
                snprintf (buffer, 512, RM " %s", &input[i][0]);
01341
                system (buffer);
01342
01343
          }
        snprintf (buffer, 512, RM " %s %s", output, result);
01344
01345
        system (buffer);
01346 #endif
01347
01348 #if DEBUG
       fprintf (stderr, "calibrate_parse: end\n");
01349
01350 #endif
01351
        // Returning the objective function
01352
01353
        return e * calibrate->weight[experiment];
01354 }
01355
01360 void
01361 calibrate print ()
01362 {
01363
       unsigned int i;
01364
        char buffer[512];
01365 #if HAVE_MPI
01366 if (calibrate->mpi_rank)
01367
          return;
01368 #endif
01369
       printf ("%s\n", gettext ("Best result"));
        fprintf (calibrate->file_result, "%s\n", gettext ("Best result"));
printf ("error = %.15le\n", calibrate->error_old[0]);
01370
01371
01372
        fprintf (calibrate->file_result, "error = %.15le\n", calibrate->
      error_old[0]);
01373
        for (i = 0; i < calibrate->nvariables; ++i)
01374
01375
            snprintf (buffer, 512, "%s = %s\n",
01376
                       calibrate->label[i], format[calibrate->precision[i]]);
01377
            printf (buffer, calibrate->value_old[i]);
            fprintf (calibrate->file_result, buffer, calibrate->value_old[i]);
01378
01379
01380
        fflush (calibrate->file_result);
01381 }
01382
01391 void
01392 calibrate_save_variables (unsigned int simulation, double error)
01393 {
01394
        unsigned int i;
01395
        char buffer[64];
01396 #if DEBUG
        fprintf (stderr, "calibrate_save_variables: start\n");
01397
01398 #endif
01399
        for (i = 0; i < calibrate->nvariables; ++i)
01400
01401
            snprintf (buffer, 64, "%s ", format[calibrate->precision[i]]);
01402
            fprintf (calibrate->file_variables, buffer,
01403
                      calibrate->value[simulation * calibrate->nvariables + i]);
01404
01405
        fprintf (calibrate->file_variables, "%.14le\n", error);
```

```
01406 #if DEBUG
       fprintf (stderr, "calibrate_save_variables: end\n");
01408 #endif
01409 }
01410
01419 void
01420 calibrate_best (unsigned int simulation, double value)
01421 {
01422
        unsigned int i, j;
        double e;
01423
01424 #if DEBUG
01425 fprintf (stderr, "calibrate_best: start\n");
01426 fprintf (stderr, "calibrate_best: nsaveds=%u nbest=%u\n",
01427
                  calibrate->nsaveds, calibrate->nbest);
01428 #endif
01429
       if (calibrate->nsaveds < calibrate->nbest
01430
             || value < calibrate->error_best[calibrate->nsaveds - 1])
          {
01431
01432
            if (calibrate->nsaveds < calibrate->nbest)
01433
               ++calibrate->nsaveds;
             calibrate->error_best[calibrate->nsaveds - 1] = value;
calibrate->simulation_best[calibrate->nsaveds - 1] = simulation;
01434
01435
01436
             for (i = calibrate->nsaveds; --i;)
01437
01438
                 if (calibrate->error_best[i] < calibrate->error_best[i - 1])
01439
                   {
01440
                      j = calibrate->simulation_best[i];
01441
                      e = calibrate->error_best[i];
01442
                      calibrate->simulation_best[i] = calibrate->
      simulation_best[i - 1];
01443
                     calibrate->error_best[i] = calibrate->error_best[i - 1];
                     calibrate->simulation_best[i - 1] = j;
calibrate->error_best[i - 1] = e;
01444
01445
01446
01447
                 else
01448
                   break:
01449
               }
01450
01451 #if DEBUG
01452 fprintf (stderr, "calibrate_best: end\n");
01453 #endif
01454 }
01455
01460 void
01461 calibrate_sequential ()
01462 {
01463 unsigned int i, j;
01464
        double e;
01465 #if DEBUG
01466 fprintf (stderr, "calibrate_sequential: start\n");
01467 fprintf (stderr, "calibrate_sequential: nstart=%u nend=%u\n",
01468
                  calibrate->nstart, calibrate->nend);
01469 #endif
01470
        for (i = calibrate->nstart; i < calibrate->nend; ++i)
01471
01472
             e = 0.;
             for (j = 0; j < calibrate->nexperiments; ++j)
01474
              e += calibrate_parse (i, j);
01475
             calibrate_best (i, e);
01476
             calibrate_save_variables (i, e);
01477 #if DEBUG
             fprintf (stderr, "calibrate_sequential: i=%u = %lg\n", i, e);
01478
01479 #endif
01480 }
01481 #if DEBUG
01482
       fprintf (stderr, "calibrate_sequential: end\n");
01483 #endif
01484 }
01485
01493 void *
01494 calibrate_thread (ParallelData * data)
01495 {
01496
        unsigned int i, j, thread;
01497
        double e;
01498 #if DEBUG
        fprintf (stderr, "calibrate_thread: start\n");
01499
01500 #endif
01501
        thread = data->thread;
01502 #if DEBUG
01503 fprintf (stderr, "calibrate_thread: thread=%u start=%u end=%u\n", thread,
                  calibrate->thread[thread], calibrate->thread[thread + 1]);
01504
01505 #endif
       for (i = calibrate->thread[thread]; i < calibrate->thread[thread + 1]; ++i)
01506
01507
            e = 0.;
01508
             for (j = 0; j < calibrate->nexperiments; ++j)
  e += calibrate_parse (i, j);
01509
01510
```

```
g_mutex_lock (mutex);
01512
           calibrate_best (i, e);
01513
           calibrate_save_variables (i, e);
01514
           g_mutex_unlock (mutex);
01515 #if DEBUG
           fprintf (stderr, "calibrate_thread: i=%u e=%lg\n", i, e);
01516
01517 #endif
01518
01519 #if DEBUG
      fprintf (stderr, "calibrate_thread: end\n");
01520
01521 #endif
01522 g_thread_exit (NULL);
01523
       return NULL;
01524 }
01525
01537 void
01538 calibrate_merge (unsigned int nsaveds, unsigned int *simulation_best,
01539
                      double *error best)
01540 {
01541
       unsigned int i, j, k, s[calibrate->nbest];
01542
       double e[calibrate->nbest];
01543 #if DEBUG
       fprintf (stderr, "calibrate_merge: start\n");
01544
01545 #endif
01546
       i = j = k = 0;
01547
       do
01548
         {
01549
           if (i == calibrate->nsaveds)
01550
             {
01551
               s[k] = simulation best[i];
01552
               e[k] = error best[i];
01553
               ++j;
01554
               ++k;
01555
               if (j == nsaveds)
01556
                 break;
01557
01558
           else if (j == nsaveds)
01559
01560
               s[k] = calibrate->simulation_best[i];
01561
               e[k] = calibrate->error_best[i];
01562
               ++i;
01563
               ++k:
               if (i == calibrate->nsaveds)
01564
01565
                 break;
01566
01567
           else if (calibrate->error_best[i] > error_best[j])
01568
               s[k] = simulation_best[j];
01569
               e[k] = error_best[j];
01570
01571
               ++i;
01572
               ++k;
01573
01574
           else
01575
             {
01576
               s[k] = calibrate->simulation best[i];
01577
               e[k] = calibrate->error best[i];
01578
               ++i;
01579
               ++k;
01580
01581
         }
       while (k < calibrate->nbest);
01582
       calibrate->nsaveds = k;
01583
       memcpy (calibrate->simulation_best, s, k * sizeof (unsigned int));
       memcpy (calibrate->error_best, e, k * sizeof (double));
01585
01586 #if DEBUG
01587
       fprintf (stderr, "calibrate_merge: end\n");
01588 #endif
01589 }
01590
01595 #if HAVE_MPI
01596 void
01597 calibrate_synchronise ()
01598 {
       unsigned int i, nsaveds, simulation_best[calibrate->nbest];
01599
       double error_best[calibrate->nbest];
01600
01601
       MPI_Status mpi_stat;
01602 #if DEBUG
01603
       fprintf (stderr, "calibrate_synchronise: start\n");
01604 #endif
01605
       if (calibrate->mpi rank == 0)
01606
01607
           for (i = 1; i < ntasks; ++i)</pre>
01608
01609
               MPI_Recv (&nsaveds, 1, MPI_INT, i, 1, MPI_COMM_WORLD, &mpi_stat);
               01610
01611
01612
               MPI_Recv (error_best, nsaveds, MPI_DOUBLE, i, 1,
```

```
MPI_COMM_WORLD, &mpi_stat);
                calibrate_merge (nsaveds, simulation_best, error_best);
01614
01615
              }
01616
          }
01617
        else
01618
            MPI_Send (&calibrate->nsaveds, 1, MPI_INT, 0, 1, MPI_COMM_WORLD);
01619
01620
            MPI_Send (calibrate->simulation_best, calibrate->nsaveds, MPI_INT, 0, 1,
01621
                       MPI_COMM_WORLD);
01622
            MPI_Send (calibrate->error_best, calibrate->nsaveds, MPI_DOUBLE, 0, 1,
                       MPI_COMM_WORLD);
01623
01624
01625 #if DEBUG
01626
       fprintf (stderr, "calibrate_synchronise: end\n");
01627 #endif
01628
01629 #endif
01630
01635 void
01636 calibrate_sweep ()
01637 {
01638
       unsigned int i, j, k, l;
01639
       double e;
        GThread *thread[nthreads];
01640
01641
        ParallelData data[nthreads];
01642 #if DEBUG
01643
        fprintf (stderr, "calibrate_sweep: start\n");
01644 #endif
        for (i = 0; i < calibrate->nsimulations; ++i)
01645
01646
01647
            k = i;
01648
             for (j = 0; j < calibrate->nvariables; ++j)
01649
01650
                1 = k % calibrate->nsweeps[j];
                 k /= calibrate->nsweeps[j];
01651
01652
                 e = calibrate->rangemin[j];
                if (calibrate->nsweeps[j] > 1)
01653
01654
                 e += 1 * (calibrate->rangemax[j] - calibrate->rangemin[j])
01655
                    / (calibrate->nsweeps[j] - 1);
01656
                calibrate->value[i * calibrate->nvariables + j] = e;
01657
              }
01658
        calibrate->nsaveds = 0;
01659
01660
        if (nthreads <= 1)</pre>
          calibrate_sequential ();
01661
01662
        else
01663
01664
            for (i = 0; i < nthreads; ++i)</pre>
01665
              {
                data[i].thread = i;
01666
01667
                thread[i]
01668
                  = g_thread_new (NULL, (void (*)) calibrate_thread, &data[i]);
01669
01670
            for (i = 0; i < nthreads; ++i)</pre>
01671
              g_thread_join (thread[i]);
01672
01673 #if HAVE_MPI
01674 // Communicating tasks results
01675 calibrate_synchronise ();
01676 #endif
01677 #if DEBUG
01678 fprintf (stderr, "calibrate_sweep: end\n");
01679 #endif
01680 }
01681
01686 void
01687 calibrate_MonteCarlo ()
01688 {
01689
        unsigned int i, i:
        GThread *thread[nthreads];
01691
        ParallelData data[nthreads];
01692 #if DEBUG
01693
        fprintf (stderr, "calibrate_MonteCarlo: start\n");
01694 #endif
        for (i = 0; i < calibrate->nsimulations; ++i)
01695
         for (j = 0; j < calibrate->nvariables; ++j)
01696
01697
            calibrate->value[i * calibrate->nvariables + j]
             = calibrate->rangemin[j] + gsl_rng_uniform (calibrate->rng)
* (calibrate->rangemax[j] - calibrate->rangemin[j]);
01698
01699
01700
        calibrate->nsaveds = 0:
01701
        if (nthreads <= 1)</pre>
01702
          calibrate_sequential ();
01703
        else
01704
            for (i = 0; i < nthreads; ++i)</pre>
01705
01706
01707
                data[i].thread = i;
```

```
thread[i]
                   = g_thread_new (NULL, (void (*)) calibrate_thread, &data[i]);
01709
01710
01711
             for (i = 0; i < nthreads; ++i)</pre>
01712
              g_thread_join (thread[i]);
01713
01714 #if HAVE_MPI
01715 // Communicating tasks results
01716 calibrate_synchronise ();
01717 #endif
01718 #if DEBUG
       fprintf (stderr, "calibrate_MonteCarlo: end\n");
01719
01720 #endif
01721 }
01722
01732 void
01733 calibrate_best_gradient (unsigned int simulation, double value)
01734 {
01735 #if DEBUG
01736
      fprintf (stderr, "calibrate_best_gradient: start\n");
01737
        fprintf (stderr,
01738
                   "calibrate_best_gradient: simulation=%u value=%.14le best=%.14le\n",
01739
                  simulation, value, calibrate->error_best[0]);
01740 #endif
01741 if (value < calibrate->error_best[0])
01742
01743
             calibrate->error_best[0] = value;
01744
             calibrate->simulation_best[0] = simulation;
01745 #if DEBUG
01746
            fprintf (stderr,
01747
                       "calibrate_best_gradient: BEST simulation=%u value=%.14le\n",
01748
                      simulation, value);
01749 #endif
01750
01751 #if DEBUG
        fprintf (stderr, "calibrate_best_gradient: end\n");
01752
01753 #endif
01754 }
01755
01762 void
01763 calibrate_gradient_sequential (unsigned int simulation)
01764 {
01765
        unsigned int i, j, k;
01766
        double e;
01767 #if DEBUG
01768 fprintf (stderr, "calibrate_gradient_sequential: start\n");
01769 fprintf (stderr, "calibrate_gradient_sequential: nstart_gradient=%u "
01770
                  "nend_gradient=%u\n",
                  calibrate->nstart_gradient, calibrate->nend_gradient);
01771
01772 #endif
01773
        for (i = calibrate->nstart_gradient; i < calibrate->nend_gradient; ++i)
01774
01775
            k = simulation + i;
             e = 0.;
01776
             for (j = 0; j < calibrate->nexperiments; ++j)
01777
             e += calibrate_parse (k, j);
calibrate_best_gradient (k, e);
01778
01779
01780
             calibrate_save_variables (k, e);
01781 #if DEBUG
01782
            fprintf (stderr, "calibrate_gradient_sequential: i=%u e=%lg\n", i, e);
01783 #endif
01784
01785 #if DEBUG
01786
       fprintf (stderr, "calibrate_gradient_sequential: end\n");
01787 #endif
01788 }
01789
01797 void *
01798 calibrate_gradient_thread (ParallelData * data)
01799 {
01800
       unsigned int i, j, thread;
01801
        double e;
01802 #if DEBUG
        fprintf (stderr, "calibrate_gradient_thread: start\n");
01803
01804 #endif
        thread = data->thread;
01805
01806 #if DEBUG
01807 fprintf (stderr, "calibrate_gradient_thread: thread=%u start=%u end=%u\n",
01808
                  thread,
                  calibrate->thread_gradient[thread],
calibrate->thread_gradient[thread + 1]);
01809
01810
01811 #endif
01812
        for (i = calibrate->thread_gradient[thread];
01813
              i < calibrate->thread_gradient[thread + 1]; ++i)
01814
            e = 0.;
01815
             for (j = 0; j < calibrate->nexperiments; ++j)
01816
```

```
e += calibrate_parse (i, j);
           g_mutex_lock (mutex);
01818
01819
            calibrate_best_gradient (i, e);
01820
            calibrate_save_variables (i, e);
01821
            g_mutex_unlock (mutex);
01822 #if DEBUG
01823
            fprintf (stderr, "calibrate_gradient_thread: i=%u e=%lg\n", i, e);
01824 #endif
01825
01826 #if DEBUG
       fprintf (stderr, "calibrate_gradient_thread: end\n");
01827
01828 #endif
01829
       g thread exit (NULL);
01830
       return NULL;
01831 }
01832
01842 double
01843 calibrate_estimate_gradient_random (unsigned int variable,
01844
                                           unsigned int estimate)
01845 {
01846
        double x;
01847 #if DEBUG
       fprintf (stderr, "calibrate_estimate_gradient_random: start\n");
01848
01849 #endif
01850 x = calibrate->gradient[variable]
          + (1. - 2. * gsl_rng_uniform (calibrate->rng)) * calibrate->step[variable];
01852 #if DEBUG
01853 fprintf (stderr, "calibrate_estimate_gradient_random: gradient%u=%lg\n",
       variable, x);
fprintf (stderr, "calibrate_estimate_gradient_random: end\n");
01854
01855
01856 #endif
01857
       return x;
01858 }
01859
01869 double
01870 calibrate_estimate_gradient_coordinates (unsigned int variable,
01871
                                                unsigned int estimate)
01872 {
01873
        double x:
01874 #if DEBUG
       fprintf \ (stderr, \ "calibrate_estimate_gradient_coordinates: \ start \ "); \\
01875
01876 #endif
01877 x = calibrate->gradient[variable];
        if (estimate >= (2 * variable) && estimate < (2 * variable + 2))</pre>
01878
01879
01880
            if (estimate & 1)
01881
             x += calibrate->step[variable];
01882
            else
01883
              x -= calibrate->step[variable];
01884
01885 #if DEBUG
01886 fprintf (stderr, "calibrate_estimate_gradient_coordinates: gradient%u=%lg\n",
01887 variable, x);
01888 fprintf (stderr, "calibrate_estimate_gradient_coordinates: end\n");
01889 #endif
01890
       return x;
01891 }
01892
01899 void
01900 calibrate_step_gradient (unsigned int simulation)
01901 {
01902
       GThread *thread[nthreads gradient];
01903
       ParallelData data[nthreads_gradient];
01904
        unsigned int i, j, k, b;
01905 #if DEBUG
01906
       fprintf (stderr, "calibrate_step_gradient: start\n");
01907 #endif
01908
       for (i = 0; i < calibrate->nestimates; ++i)
01909
            k = (simulation + i) * calibrate->nvariables;
01911
            b = calibrate->simulation_best[0] * calibrate->nvariables;
01912 #if DEBUG
01913
           fprintf (stderr, "calibrate_step_gradient: simulation=%u best=%u\n",
                     simulation + i, calibrate->simulation_best[0]);
01914
01915 #endif
01916
           for (j = 0; j < calibrate->nvariables; ++j, ++k, ++b)
01917
01918 #if DEBUG
01919
                fprintf (stderr,
                          "calibrate_step_gradient: estimate=%u best%u=%.14le\n",
01920
01921
                         i, j, calibrate->value[b]);
01922 #endif
01923
               calibrate->value[k]
01924
                  = calibrate->value[b] + calibrate_estimate_gradient (j, i);
01925
                calibrate->value[k] = fmin (fmax (calibrate->value[k],
                                                   calibrate->rangeminabs[j]),
01926
01927
                                             calibrate->rangemaxabs[i]);
```

```
01928 #if DEBUG
01929
               fprintf (stderr,
01930
                         "calibrate_step_gradient: estimate=%u variable%u=%.14le\n",
                         i, j, calibrate->value[k]);
01931
01932 #endif
01933
01934
01935
        if (nthreads_gradient == 1)
01936
         calibrate_gradient_sequential (simulation);
01937
        else
        {
01938
01939
           for (i = 0; i <= nthreads_gradient; ++i)</pre>
01940
01941
                calibrate->thread_gradient[i]
01942
                  = simulation + calibrate->nstart_gradient
                  + i * (calibrate->nend_gradient - calibrate->
01943
     nstart_gradient)
01944
                 / nthreads_gradient;
01945 #if DEBUG
01946
               fprintf (stderr,
01947
                         "calibrate_step_gradient: i=%u thread_gradient=%u\n",
01948
                         i, calibrate->thread_gradient[i]);
01949 #endif
01950
              }
01951
            for (i = 0; i < nthreads_gradient; ++i)</pre>
01952
01953
                data[i].thread = i;
01954
                thread[i] = g_thread_new
01955
                  (NULL, (void (*)) calibrate_gradient_thread, &data[i]);
01956
01957
            for (i = 0; i < nthreads_gradient; ++i)</pre>
01958
             g_thread_join (thread[i]);
01959
01960 #if DEBUG
01961 fprintf (stderr, "calibrate_step_gradient: end\n");
01962 #endif
01963 }
01964
01969 void
01970 calibrate_gradient ()
01971 {
01972
       unsigned int i, j, k, b, s, adjust;
01973 #if DEBUG
01974
       fprintf (stderr, "calibrate_gradient: start\n");
01975 #endif
01976
       for (i = 0; i < calibrate->nvariables; ++i)
01977
         calibrate->gradient[i] = 0.;
       b = calibrate->simulation_best[0] * calibrate->nvariables;
01978
01979
       s = calibrate->nsimulations:
01980
       adiust = 1;
       for (i = 0; i < calibrate->nsteps; ++i, s += calibrate->nestimates, b = k)
01982
01983 #if DEBUG
01984
       fprintf (stderr, "calibrate_gradient: step=%u old_best=%u\n",
                     i, calibrate->simulation_best[0]);
01985
01986 #endif
       calibrate_step_gradient (s);
           k = calibrate->simulation_best[0] * calibrate->nvariables;
01988
01989 #if DEBUG
           fprintf (stderr, "calibrate_gradient: step=%u best=%u\n",
01990
                     i, calibrate->simulation_best[0]);
01991
01992 #endif
01993
           if (k == b)
01994
                if (adjust)
01995
01996
                 for (j = 0; j < calibrate->nvariables; ++j)
                   calibrate->step[j] *= 0.5;
01997
                for (j = 0; j < calibrate->nvariables; ++j)
  calibrate->gradient[j] = 0.;
01998
01999
02000
                adjust = 1;
02001
02002
            else
02003
             {
02004
                for (j = 0; j < calibrate->nvariables; ++j)
02005
02006 #if DEBUG
02007
                    fprintf (stderr,
02008
                              "calibrate_gradient: best%u=%.14le old%u=%.14le\n",
02009
                             j, calibrate->value[k + j], j, calibrate->value[b + j]);
02010 #endif
                    calibrate->gradient[i]
02011
02012
                     = (1. - calibrate->relaxation) * calibrate->gradient[j]
02013
                      + calibrate->relaxation
02014
                      * (calibrate->value[k + j] - calibrate->value[b + j]);
02015 #if DEBUG
                    fprintf (stderr, "calibrate_gradient: gradient%u=%.14le\n",
02016
                             j, calibrate->gradient[j]);
02017
```

```
02018 #endif
02019
02020
               adjust = 0;
              }
02021
02022
02023 #if DEBUG
02024 fprintf (stderr, "calibrate_gradient: end\n");
02025 #endif
02026 }
02027
02035 double
02036 calibrate_genetic_objective (Entity * entity)
02037 {
02038
       unsigned int j;
02039
        double objective;
02040
       char buffer[64];
02041 #if DEBUG
02042
       fprintf (stderr, "calibrate genetic objective: start\n");
02043 #endif
02044
       for (j = 0; j < calibrate->nvariables; ++j)
02045
02046
            calibrate->value[entity->id * calibrate->nvariables + j]
              = genetic_get_variable (entity, calibrate->genetic_variable + j);
02047
02048
02049
        for (j = 0, objective = 0.; j < calibrate->nexperiments; ++j)
         objective += calibrate_parse (entity->id, j);
02050
        g_mutex_lock (mutex);
02051
        for (j = 0; j < calibrate->nvariables; ++j)
02052
02053
            snprintf (buffer, 64, "%s ", format[calibrate->precision[j]]);
02054
            fprintf (calibrate->file_variables, buffer,
02055
02056
                     genetic_get_variable (entity, calibrate->genetic_variable + j));
02057
02058
       fprintf (calibrate->file_variables, "%.14le\n", objective);
        g_mutex_unlock (mutex);
02059
02060 #if DEBUG
02061
       fprintf (stderr, "calibrate genetic objective: end\n");
02062 #endif
02063
       return objective;
02064 }
02065
02070 void
02071 calibrate_genetic ()
02072 {
02073
        char *best_genome;
02074
        double best_objective, *best_variable;
02075 #if DEBUG
       fprintf (stderr, "calibrate_genetic: start\n");
fprintf (stderr, "calibrate_genetic: ntasks=%u nthreads=%u\n", ntasks,
02076
02077
02078
                 nthreads):
       fprintf (stderr,
02080
                  "calibrate_genetic: nvariables=%u population=%u generations=%u\n",
02081
                 calibrate->nvariables, calibrate->nsimulations,
02082
                 calibrate->niterations);
02083
       fprintf (stderr,
                  "calibrate_genetic: mutation=%lg reproduction=%lg adaptation=%lg\n",
02084
                 calibrate->mutation_ratio, calibrate->
     reproduction_ratio,
02086
                 calibrate->adaptation_ratio);
02087 #endif
02088
       genetic algorithm default (calibrate->nvariables,
02089
                                    calibrate->genetic variable,
02090
                                    calibrate->nsimulations,
02091
                                    calibrate->niterations,
02092
                                    calibrate->mutation_ratio,
02093
                                    calibrate->reproduction_ratio,
02094
                                    calibrate->adaptation_ratio,
02095
                                    &calibrate genetic objective.
02096
                                    &best genome, &best variable, &best objective);
02098
        fprintf (stderr, "calibrate_genetic: the best\n");
02099 #endif
02100
       calibrate->error_old = (double *) g_malloc (sizeof (double));
02101
        calibrate->value old
            (double *) g_malloc (calibrate->nvariables * sizeof (double));
02102
02103
       calibrate->error_old[0] = best_objective;
02104
       memcpy (calibrate->value_old, best_variable,
02105
                calibrate->nvariables * sizeof (double));
02106
       g_free (best_genome);
02107
       g_free (best_variable);
        calibrate_print ();
02108
02109 #if DEBUG
02110
       fprintf (stderr, "calibrate_genetic: end\n");
02111 #endif
02112 }
02113
02118 void
```

```
02119 calibrate_save_old ()
02120 {
02121
       unsigned int i, j;
02122 #if DEBUG
02123 fprintf (stderr, "calibrate_save_old: start\n");
02124 fprintf (stderr, "calibrate_save_old: nsaveds=%u\n", calibrate->nsaveds);
02125 #endif
02126 memcpy (calibrate->error_old, calibrate->error_best,
               calibrate->nbest * sizeof (double));
02127
       for (i = 0; i < calibrate->nbest; ++i)
02128
02129
       {
            j = calibrate->simulation_best[i];
02130
02131 #if DEBUG
02132
           fprintf (stderr, "calibrate_save_old: i=%u j=%u\n", i, j);
02133 #endif
02134
       memcpy (calibrate->value_old + i * calibrate->nvariables,
                    calibrate->value + j * calibrate->nvariables,
02135
                   calibrate->nvariables * sizeof (double));
02136
02137
02138 #if DEBUG
02139 for (i = 0; i < calibrate->nvariables; ++i)
        02140
02141
       fprintf (stderr, "calibrate_save_old: end\n");
02142
02143 #endif
02144 }
02145
02151 void
02152 calibrate_merge_old ()
02153 {
02154 unsigned int i, i, k:
02155
        double v[calibrate->nbest * calibrate->nvariables], e[calibrate->
     nbest],
02156
         *enew, *eold;
02157 #if DEBUG
       fprintf (stderr, "calibrate_merge_old: start\n");
02158
02159 #endif
02160 enew = calibrate->error_best;
02161
        eold = calibrate->error_old;
02162
        i = j = k = 0;
02163
       do
02164
        {
           if (*enew < *eold)</pre>
02165
02166
             {
               memcpy (v + k * calibrate->nvariables,
02167
02168
                       calibrate->value
02169
nvariables,
                       + calibrate->simulation_best[i] * calibrate->
                       calibrate->nvariables * sizeof (double));
02171
               e[k] = *enew;
               ++k;
02173
               ++enew;
02174
               ++i;
02175
02176
           else
02177
             {
02178
               memcpy (v + k * calibrate->nvariables,
02179
                        calibrate->value_old + j * calibrate->nvariables,
02180
                        calibrate->nvariables * sizeof (double));
02181
               e[k] = *eold;
02182
               ++k:
02183
               ++eold;
02184
               ++j;
02185
02186
02187
       while (k < calibrate->nbest);
      memcpy (calibrate->value_old, v, k * calibrate->nvariables * sizeof (double));
02188
02189
       memcpy (calibrate->error_old, e, k * sizeof (double));
02190 #if DEBUG
02191
       fprintf (stderr, "calibrate_merge_old: end\n");
02192 #endif
02193 }
02194
02200 void
02201 calibrate_refine ()
02202 {
02203 unsigned int i, j;
02204 double d;
02205 #if HAVE_MPI
      MPI_Status mpi_stat;
02206
02207 #endif
02208 #if DEBUG
02209
       fprintf (stderr, "calibrate_refine: start\n");
02210 #endif
02211 #if HAVE_MPI
02212
      if (!calibrate->mpi_rank)
02213
```

```
02214 #endif
           for (j = 0; j < calibrate->nvariables; ++j)
02215
02216
                calibrate->rangemin[j] = calibrate->rangemax[j]
02217
02218
                 = calibrate->value_old[j];
02219
02220
            for (i = 0; ++i < calibrate->nbest;)
02221
02222
                for (j = 0; j < calibrate->nvariables; ++j)
02223
02224
                   calibrate->rangemin[j]
02225
                     = fmin (calibrate->rangemin[j],
                             calibrate->value_old[i * calibrate->nvariables + j]);
02226
                   calibrate->rangemax[j]
02227
02228
                     = fmax (calibrate->rangemax[j],
02229
                             calibrate->value_old[i * calibrate->nvariables + j]);
02230
                 }
02231
02232
           for (j = 0; j < calibrate->nvariables; ++j)
02233
02234
                d = calibrate->tolerance
02235
                 * (calibrate->rangemax[j] - calibrate->rangemin[j]);
                switch (calibrate->algorithm)
02236
02237
02238
                 case ALGORITHM_MONTE_CARLO:
                  d *= 0.5;
02239
02240
                   break;
02241
                 default:
02242
                   if (calibrate->nsweeps[j] > 1)
                     d /= calibrate->nsweeps[j] - 1;
02243
02244
                   else
                     d = 0.;
02245
02246
02247
                calibrate->rangemin[j] -= d;
02248
               calibrate->rangemin[j]
02249
                 = fmax (calibrate->rangemin[j], calibrate->rangeminabs[j]);
                calibrate->rangemax[j] += d;
02250
               calibrate->rangemax[j]
02252
                 = fmin (calibrate->rangemax[j], calibrate->rangemaxabs[j]);
02253
               printf ("%s min=%lg max=%lg\n", calibrate->label[j],
               02254
02255
02256
02257
                        calibrate->rangemax[j]);
02258
02259 #if HAVE_MPI
02260
       for (i = 1; i < ntasks; ++i)</pre>
02261
               MPI_Send (calibrate->rangemin, calibrate->nvariables, MPI_DOUBLE, i,
02262
02263
                         1, MPI_COMM_WORLD);
               MPI_Send (calibrate->rangemax, calibrate->nvariables, MPI_DOUBLE, i,
02264
02265
                         1, MPI_COMM_WORLD);
02266
02267
         }
02268
       else
02269
        {
           MPI_Recv (calibrate->rangemin, calibrate->nvariables, MPI_DOUBLE, 0, 1,
02271
                     MPI_COMM_WORLD, &mpi_stat);
02272
            MPI_Recv (calibrate->rangemax, calibrate->nvariables, MPI_DOUBLE, 0, 1,
02273
                     MPI_COMM_WORLD, &mpi_stat);
02274
02275 #endif
02276 #if DEBUG
02277
       fprintf (stderr, "calibrate_refine: end\n");
02278 #endif
02279 }
02280
02285 void
02286 calibrate_step ()
02288 #if DEBUG
       fprintf (stderr, "calibrate_step: start\n");
02289
02290 #endif
02291 calibrate_algorithm ();
       if (calibrate->nsteps)
02292
         calibrate_gradient ();
02293
02294 #if DEBUG
02295 fprintf (stderr, "calibrate_step: end\n"); 02296 #endif
02297 }
02298
02303 void
02304 calibrate_iterate ()
02305 {
02306
       unsigned int i;
02307 #if DEBUG
02308 fprintf (stderr, "calibrate_iterate: start\n");
```

```
02309 #endif
02310
       calibrate->error_old
02311
          = (double *) g_malloc (calibrate->nbest * sizeof (double));
        calibrate->value_old = (double *)
02312
         g_malloc (calibrate->nbest * calibrate->nvariables * sizeof (double));
02313
       calibrate_step ();
calibrate_save_old ();
02314
02315
02316
        calibrate_refine ();
02317
        calibrate_print ();
02318
        for (i = 1; i < calibrate->niterations; ++i)
02319
02320
            calibrate_step ();
02321
            calibrate_merge_old ();
02322
            calibrate_refine ();
02323
            calibrate_print ();
02324
02325 #if DEBUG
       fprintf (stderr, "calibrate_iterate: end\n");
02326
02327 #endif
02328 }
02329
02334 void
02335 calibrate_free ()
02336 {
02337
        unsigned int i, j;
02338 #if DEBUG
02339
        fprintf (stderr, "calibrate_free: start\n");
02340 #endif
       for (j = 0; j < calibrate->ninputs; ++j)
02341
02342
02343
            for (i = 0; i < calibrate->nexperiments; ++i)
            g_mapped_file_unref (calibrate->file[j][i]);
g_free (calibrate->file[j]);
02344
02345
02346
02347
        g_free (calibrate->error_old);
02348
        g_free (calibrate->value_old);
       g_free (calibrate->value);
02349
       g_free (calibrate->genetic_variable);
02350
02351
        g_free (calibrate->rangemax);
02352
        g_free (calibrate->rangemin);
02353 #if DEBUG
02354
       fprintf (stderr, "calibrate free: end\n");
02355 #endif
02356 }
02357
02362 void
02363 calibrate_open ()
02364 {
02365
        GTimeZone *tz:
02366
       GDateTime *t0, *t;
       unsigned int i, j, *nbits;
02367
02368
02369 #if DEBUG
      char *buffer;
02370
       fprintf (stderr, "calibrate_open: start\n");
02371
02372 #endif
02373
02374
        // Getting initial time
02375 #if DEBUG
       fprintf (stderr, "calibrate_open: getting initial time\n");
02376
02377 #endif
02378 tz = g_time_zone_new_utc ();
02379
       t0 = g_date_time_new_now (tz);
02380
02381
        // Obtaining and initing the pseudo-random numbers generator seed
02382 #if DEBUG
       fprintf (stderr, "calibrate_open: getting initial seed\n");
02383
02384 #endif
02385 calibrate->seed = input->seed;
       gsl_rng_set (calibrate->rng, calibrate->seed);
02386
02387
02388
       // Replacing the working directory
02389 #if DEBUG
       fprintf (stderr, "calibrate_open: replacing the working directory\n");
02390
02391 #endif
02392
       g_chdir (input->directory);
02393
02394
        // Getting results file names
02395
       calibrate->result = input->result;
       calibrate->variables = input->variables;
02396
02397
02398
        // Obtaining the simulator file
02399
        calibrate->simulator = input->simulator;
02400
02401
        \ensuremath{//} Obtaining the evaluator file
02402
        calibrate->evaluator = input->evaluator;
02403
```

```
// Reading the algorithm
        calibrate->algorithm = input->algorithm;
02405
02406
        switch (calibrate->algorithm)
02407
         case ALGORITHM MONTE CARLO:
02408
          calibrate_algorithm = calibrate_MonteCarlo;
break;
02409
02410
02411
          case ALGORITHM_SWEEP:
          calibrate_algorithm = calibrate_sweep;
02412
           break;
02413
02414
         default:
02415
          calibrate algorithm = calibrate genetic;
02416
            calibrate->mutation_ratio = input->mutation_ratio;
            calibrate->reproduction_ratio = input->
     reproduction_ratio;
02418
           calibrate->adaptation_ratio = input->adaptation_ratio;
02419
02420
       calibrate->nvariables = input->nvariables;
       calibrate->nsimulations = input->nsimulations;
02421
        calibrate->niterations = input->niterations;
02422
02423
        calibrate->nbest = input->nbest;
02424
        calibrate->tolerance = input->tolerance;
02425
        calibrate->nsteps = input->nsteps;
        calibrate->nestimates = 0;
02426
02427
        if (input->nsteps)
02428
        {
02429
            calibrate->gradient_method = input->gradient_method;
02430
            calibrate->relaxation = input->relaxation;
02431
            switch (input->gradient_method)
02432
             {
02433
             case GRADIENT_METHOD_COORDINATES:
02434
               calibrate->nestimates = 2 * calibrate->nvariables;
                calibrate_estimate_gradient =
02435
     calibrate_estimate_gradient_coordinates;
02436
               break;
02437
              default:
02438
               calibrate->nestimates = input->nestimates;
               calibrate_estimate_gradient =
02439
     calibrate_estimate_gradient_random;
02440
02441
02442
02443 #if DEBUG
02444
       fprintf (stderr, "calibrate_open: nbest=%u\n", calibrate->nbest);
02446 calibrate->simulation_best
02447
         = (unsigned int *) alloca (calibrate->nbest * sizeof (unsigned int));
02448
       calibrate->error best
         = (double *) alloca (calibrate->nbest * sizeof (double));
02449
02450
02451
        // Reading the experimental data
02452 #if DEBUG
02453 buffer = g_get_current_dir ();
02454
        fprintf (stderr, "calibrate_open: current directory=%sn", buffer);
02455
        g_free (buffer);
02456 #endif
02457
       calibrate->nexperiments = input->nexperiments;
02458
        calibrate->ninputs = input->ninputs;
02459
        calibrate->experiment = input->experiment;
02460
        calibrate->weight = input->weight;
02461
        for (i = 0; i < input->ninputs; ++i)
02462
02463
            calibrate->template[i] = input->template[i];
02464
            calibrate->file[i]
02465
              = g_malloc (input->nexperiments * sizeof (GMappedFile *));
02466
02467
       for (i = 0; i < input->nexperiments; ++i)
02468
02469 #if DEBUG
            fprintf (stderr, "calibrate_open: i=%u\n", i);
fprintf (stderr, "calibrate_open: experiment=%s\n",
02471
02472
                     calibrate->experiment[i]);
02473
            02474 #endif
02475
            for (j = 0; j < input->ninputs; ++j)
02476
02477 #if DEBUG
           fprintf (stderr, "calibrate_open: template%u\n", j + 1);
fprintf (stderr, "calibrate_open: experiment=%u template%u=%s\n",
02478
02479
                         i, j + 1, calibrate->template[j][i]);
02480
02481 #endif
02482
               calibrate->file[j][i]
02483
                  = g_mapped_file_new (input->template[j][i], 0, NULL);
02484
             }
02485
        }
02486
02487
       // Reading the variables data
```

```
02488 #if DEBUG
        fprintf (stderr, "calibrate_open: reading variables\n");
02489
02490 #endif
02491
        calibrate->label = input->label;
        j = input->nvariables * sizeof (double);
calibrate->rangemin = (double *) g_malloc (j);
calibrate->rangemax = (double *) g_malloc (j);
02492
02493
02494
02495
        memcpy (calibrate->rangemin, input->rangemin, j);
02496
        memcpy (calibrate->rangemax, input->rangemax, j);
02497
        calibrate->rangeminabs = input->rangeminabs;
        calibrate->rangemaxabs = input->rangemaxabs;
02498
        calibrate->precision = input->precision;
02499
        calibrate->nsweeps = input->nsweeps;
02500
02501
        calibrate->step = input->step;
02502
        nbits = input->nbits;
02503
        if (input->algorithm == ALGORITHM_SWEEP)
02504
02505
            calibrate->nsimulations = 1;
            for (i = 0; i < input->nvariables; ++i)
02507
02508
                if (input->algorithm == ALGORITHM_SWEEP)
02509
02510
                     calibrate->nsimulations *= input->nsweeps[i];
02511 #if DEBUG
02512
                    fprintf (stderr, "calibrate_open: nsweeps=%u nsimulations=%u\n",
                              calibrate->nsweeps[i], calibrate->nsimulations);
02513
02514 #endif
02515
02516
              }
02517
          }
02518
       if (calibrate->nsteps)
02519
        calibrate->gradient
02520
            = (double *) alloca (calibrate->nvariables * sizeof (double));
02521
02522
        // Allocating values
02523 #if DEBUG
       fprintf (stderr, "calibrate_open: allocating variables\n");
fprintf (stderr, "calibrate_open: nvariables=%u\n", calibrate->nvariables);
02524
02526 #endif
02527
       calibrate->genetic_variable = NULL;
02528
        if (calibrate->algorithm == ALGORITHM_GENETIC)
02529
            calibrate->genetic variable = (GeneticVariable *)
02530
02531
              g_malloc (calibrate->nvariables * sizeof (GeneticVariable));
            for (i = 0; i < calibrate->nvariables; ++i)
02532
02533
02534 #if DEBUG
                fprintf (stderr, "calibrate_open: i=%u min=%lg max=%lg nbits=%u\n",
02535
02536
                          i, calibrate->rangemin[i], calibrate->rangemax[i], nbits[i]);
02537 #endif
02538
                calibrate->genetic_variable[i].minimum = calibrate->
      rangemin[i];
02539
                calibrate->genetic_variable[i].maximum = calibrate->
     rangemax[i];
02540
                calibrate->genetic_variable[i].nbits = nbits[i];
02541
              }
02542
02543 #if DEBUG
02544 fprintf (stderr, "calibrate_open: nvariables=%u nsimulations=%u\n",
02545
                 calibrate->nvariables, calibrate->nsimulations);
02546 #endif
02547 calibrate->value = (double *)
         g_malloc ((calibrate->nsimulations
02549
                      + calibrate->nestimates * calibrate->nsteps)
02550
                     * calibrate->nvariables * sizeof (double));
02551
        // Calculating simulations to perform on each task
02552
02553 #if HAVE_MPI
02554 #if DEBUG
       fprintf (stderr, "calibrate_open: rank=%u ntasks=%u\n",
02556
                 calibrate->mpi_rank, ntasks);
02557 #endif
02558
       calibrate->nstart = calibrate->mpi_rank * calibrate->
     nsimulations / ntasks;
      calibrate->nend
02559
          = (1 + calibrate->mpi_rank) * calibrate->nsimulations /
     ntasks;
02561 if (calibrate->nsteps)
02562
02563
            calibrate->nstart gradient
02564
              = calibrate->mpi rank * calibrate->nestimates / ntasks;
02565
            calibrate->nend_gradient
               = (1 + calibrate->mpi_rank) * calibrate->nestimates /
     ntasks;
02567
02568 #else
02569
        calibrate->nstart = 0;
```

```
calibrate->nend = calibrate->nsimulations;
02571
        if (calibrate->nsteps)
02572
02573
            calibrate->nstart gradient = 0;
            calibrate->nend_gradient = calibrate->nestimates;
02574
02575
02576 #endif
02577 #if DEBUG
02578 fprintf (stderr, "calibrate_open: nstart=%u nend=%u\n", calibrate->nstart,
02579
                 calibrate->nend);
02580 #endif
02581
02582
        // Calculating simulations to perform for each thread
02583
       calibrate->thread
02584
         = (unsigned int *) alloca ((1 + nthreads) * sizeof (unsigned int));
02585
        for (i = 0; i <= nthreads; ++i)</pre>
02586
02587
            calibrate->thread[i] = calibrate->nstart
              + i * (calibrate->nend - calibrate->nstart) / nthreads;
02588
02589 #if DEBUG
02590
            fprintf (stderr, "calibrate_open: i=%u thread=%u\n", i,
02591
                      calibrate->thread[i]);
02592 #endif
02593
02594
        if (calibrate->nsteps)
        calibrate->thread_gradient = (unsigned int *)
02595
02596
            alloca ((1 + nthreads_gradient) * sizeof (unsigned int));
02597
02598
       // Opening result files
02599
        calibrate->file_result = g_fopen (calibrate->result, "w");
02600
        calibrate->file_variables = g_fopen (calibrate->variables, "w");
02601
02602
        // Performing the algorithm
02603
        switch (calibrate->algorithm)
02604
            // Genetic algorithm
02605
         case ALGORITHM_GENETIC:
02606
           calibrate_genetic ();
02607
02608
           break:
02609
02610
            // Iterative algorithm
          default:
02611
02612
           calibrate iterate ();
02613
02614
02615
        // Getting calculation time
02616
        t = g_date_time_new_now (tz);
        calibrate->calculation_time = 0.000001 * g_date_time_difference (t, t0);
02617
        g_date_time_unref (t);
02618
02619
        q_date_time_unref (t0);
02620
        g_time_zone_unref (tz);
02621
       printf ("%s = %.61g s\n",
02622
                gettext ("Calculation time"), calibrate->calculation_time);
       fprintf (calibrate->file_result, "%s = %.6lg s\n",
    gettext ("Calculation time"), calibrate->calculation_time);
02623
02624
02625
02626 // Closing result files
02627 fclose (calibrate->file_variables);
02628 fclose (calibrate->file_result);
02629
02630 #if DEBUG
02631 fprintf (stderr, "calibrate_open: end\n");
02632 #endif
02633 }
02634
02635 #if HAVE_GTK
02636
02643 void
02644 input_save_gradient (xmlNode * node)
02645 {
02646 if (input->nsteps)
02648
            xml_node_set_uint (node, XML_NSTEPS, input->
     nsteps);
         if (input->relaxation != DEFAULT_RELAXATION)
02649
              xml_node_set_float (node, XML_RELAXATION, input->
     relaxation);
02651
         switch (input->gradient_method)
02652
              {
              case GRADIENT_METHOD_COORDINATES:
02653
                xmlSetProp (node, XML_GRADIENT_METHOD,
02654
     XML_COORDINATES);
02655
               break;
02656
               default:
02657
               xmlSetProp (node, XML_GRADIENT_METHOD, XML_RANDOM);
02658
                xml_node_set_uint (node, XML_NESTIMATES, input->
      nestimates);
```

```
}
02660
02661 }
02662
02669 void
02670 input save (char *filename)
02671 {
02672
         unsigned int i, j;
02673
         char *buffer;
02674
         xmlDoc *doc;
02675
         xmlNode *node, *child;
02676
         GFile *file, *file2;
02677
02678
         // Getting the input file directory
02679
         input->name = g_path_get_basename (filename);
         input->directory = g_path_get_dirname (filename);
02680
02681
         file = g_file_new_for_path (input->directory);
02682
02683
         // Opening the input file
02684
         doc = xmlNewDoc ((const xmlChar *) "1.0");
02685
02686
         // Setting root XML node
         node = xmlNewDocNode (doc, 0, XML_CALIBRATE, 0);
02687
02688
         xmlDocSetRootElement (doc, node);
02689
02690
         // Adding properties to the root XML node
02691
         if (xmlStrcmp ((const xmlChar *) input->result, result_name))
02692
           xmlSetProp (node, XML_RESULT, (xmlChar *) input->result);
02693
         if (xmlStrcmp ((const xmlChar *) input->variables, variables_name))
         xmlSetProp (node, XML_VARIABLES, (xmlChar *) input->variables);
file2 = g_file_new_for_path (input->simulator);
02694
02695
02696
         buffer = g_file_get_relative_path (file, file2);
02697
         g_object_unref (file2);
02698
         xmlSetProp (node, XML_SIMULATOR, (xmlChar *) buffer);
02699
         g_free (buffer);
02700
         if (input->evaluator)
02701
           {
              file2 = g_file_new_for_path (input->evaluator);
02702
02703
              buffer = g_file_get_relative_path (file, file2);
02704
              g_object_unref (file2);
02705
              if (xmlStrlen ((xmlChar *) buffer))
02706
                xmlSetProp (node, XML_EVALUATOR, (xmlChar *) buffer);
02707
              q free (buffer);
02708
02709
         if (input->seed != DEFAULT_RANDOM_SEED)
02710
            xml_node_set_uint (node, XML_SEED, input->seed);
02711
02712
         \ensuremath{//} Setting the algorithm
02713
         buffer = (char *) g_malloc (64);
02714
         switch (input->algorithm)
02715
02716
           case ALGORITHM_MONTE_CARLO:
02717
              xmlSetProp (node, XML_ALGORITHM, XML_MONTE_CARLO);
              snprintf (buffer, 64, "%u", input->nsimulations);
xmlSetProp (node, XML_NSIMULATIONS, (xmlChar *) buffer);
snprintf (buffer, 64, "%u", input->niterations);
02718
02719
02720
              xmlSetProp (node, XML_NITERATIONS, (xmlChar *) buffer);
02721
              snprintf (buffer, 64, "%.31g", input->tolerance);
xmlSetProp (node, XML_TOLERANCE, (xmlChar *) buffer);
02722
02723
              snprintf (buffer, 64, "%u", input->nbest);
xmlSetProp (node, XML_NBEST, (xmlChar *) buffer);
02724
02725
02726
              input_save_gradient (node);
              break;
02728
            case ALGORITHM_SWEEP:
02729
              xmlSetProp (node, XML_ALGORITHM, XML_SWEEP);
02730
              snprintf (buffer, 64, "%u", input->niterations);
              xmlSetProp (node, XML_NITERATIONS, (xmlChar *) buffer);
snprintf (buffer, 64, "%.3lg", input->tolerance);
02731
02732
              xmlSetProp (node, XML_TOLERANCE, (xmlChar *) buffer);
02733
              snprintf (buffer, 64, "%u", input->nbest);
xmlSetProp (node, XML_NBEST, (xmlChar *) buffer);
02735
02736
              input_save_gradient (node);
02737
              break;
02738
            default:
02739
              xmlSetProp (node, XML_ALGORITHM, XML_GENETIC);
02740
              snprintf (buffer, 64, "%u", input->nsimulations);
02741
              xmlSetProp (node, XML_NPOPULATION, (xmlChar *) buffer);
02742
              snprintf (buffer, 64, "%u", input->niterations);
              xmlSetProp (node, XML_NGENERATIONS, (xmlChar *) buffer);
snprintf (buffer, 64, "%.31g", input->mutation_ratio);
xmlSetProp (node, XML_MUTATION, (xmlChar *) buffer);
snprintf (buffer, 64, "%.31g", input->reproduction_ratio);
02743
02744
02745
02746
              xmlSetProp (node, XML_REPRODUCTION, (xmlChar *) buffer);
snprintf (buffer, 64, "%.31g", input->adaptation_ratio);
02747
02748
              xmlSetProp (node, XML_ADAPTATION, (xmlChar *) buffer);
02749
02750
              break;
02751
           }
```

```
g_free (buffer);
02753
02754
        // Setting the experimental data
02755
        for (i = 0; i < input->nexperiments; ++i)
02756
02757
            child = xmlNewChild (node, 0, XML_EXPERIMENT, 0);
            xmlSetProp (child, XML_NAME, (xmlChar *) input->experiment[i]);
02758
            if (input->weight[i] != 1.)
02759
02760
              xml_node_set_float (child, XML_WEIGHT, input->
     weight[i]);
02761
            for (j = 0; j < input->ninputs; ++j)
             xmlSetProp (child, template[j], (xmlChar *) input->template[j][i]);
02762
02763
          }
02764
02765
        // Setting the variables data
02766
        for (i = 0; i < input->nvariables; ++i)
02767
02768
            child = xmlNewChild (node, 0, XML_VARIABLE, 0);
            xmlSetProp (child, XML_NAME, (xmlChar *) input->label[i]);
            xml_node_set_float (child, XML_MINIMUM, input->
     rangemin[i]);
02771
           if (input->rangeminabs[i] != -G_MAXDOUBLE)
             xml_node_set_float (child, XML_ABSOLUTE_MINIMUM, input->
02772
      rangeminabs[i]);
02773
           xml_node_set_float (child, XML_MAXIMUM, input->
     rangemax[i]);
02774
           if (input->rangemaxabs[i] != G_MAXDOUBLE)
02775
             xml_node_set_float (child, XML_ABSOLUTE_MAXIMUM, input->
     rangemaxabs[i]);
          if (input->precision[i] != DEFAULT_PRECISION)
02776
02777
             xml_node_set_uint (child, XML_PRECISION, input->
     precision[i]);
02778
         if (input->algorithm == ALGORITHM_SWEEP)
             xml_node_set_uint (child, XML_NSWEEPS, input->
02779
     nsweeps[i]);
        else if (input->algorithm == ALGORITHM_GENETIC)
02780
              xml_node_set_uint (child, XML_NBITS, input->
02781
     nbits[i]);
02782
02783
02784
        // Saving the XML file
02785
       xmlSaveFormatFile (filename, doc, 1);
02786
02787
       // Freeing memory
02788
       xmlFreeDoc (doc);
02789 }
02790
02795 void
02796 options_new ()
02797 {
02798
       options->label_seed = (GtkLabel *)
02799
          gtk_label_new (gettext ("Pseudo-random numbers generator seed"));
        options->spin_seed = (GtkSpinButton *)
02800
02801
          gtk_spin_button_new_with_range (0., (gdouble) G_MAXULONG, 1.);
02802
        {\tt gtk\_widget\_set\_tooltip\_text}
          (GTK_WIDGET (options->spin_seed),
02803
           gettext ("Seed to init the pseudo-random numbers generator"));
02804
02805
        gtk_spin_button_set_value (options->spin_seed, (gdouble) input->seed);
02806
        options->label_threads = (GtkLabel *)
02807
          gtk_label_new (gettext ("Threads number for the stochastic algorithm"));
        options->spin threads
02808
02809
          = (GtkSpinButton *) gtk_spin_button_new_with_range (1., 64., 1.);
02810
        gtk_widget_set_tooltip_text
         (GTK_WIDGET (options->spin_threads),
02811
           gettext ("Number of threads to perform the calibration/optimization for "
02812
02813
                    "the stochastic algorithm"));
02814
        gtk_spin_button_set_value (options->spin_threads, (gdouble)
      nthreads);
02815
        options->label_gradient = (GtkLabel *)
          gtk_label_new (gettext ("Threads number for the gradient based method"));
02816
02817
        options->spin_gradient
02818
          = (GtkSpinButton *) gtk_spin_button_new_with_range (1., 64., 1.);
02819
        {\tt gtk\_widget\_set\_tooltip\_text}
02820
          (GTK_WIDGET (options->spin_gradient),
           gettext ("Number of threads to perform the calibration/optimization for "
    "the gradient based method"));
02821
02822
02823
       gtk_spin_button_set_value (options->spin_gradient,
02824
                                   (gdouble) nthreads_gradient);
        options->grid = (GtkGrid *) gtk_grid_new ();
02825
        gtk_grid_attach (options->grid, GTK_WIDGET (options->label_seed), 0, 0, 1, 1);
gtk_grid_attach (options->grid, GTK_WIDGET (options->spin_seed), 1, 0, 1, 1);
02826
02827
        gtk_grid_attach (options->grid, GTK_WIDGET (options->label_threads),
02828
02829
                         0, 1, 1, 1);
02830
        gtk_grid_attach (options->grid, GTK_WIDGET (options->spin_threads),
02831
                         1, 1, 1, 1);
       02832
02833
```

```
gtk_grid_attach (options->grid, GTK_WIDGET (options->spin_gradient),
        1, 2, 1, 1);
gtk_widget_show_all (GTK_WIDGET (options->grid));
02835
02836
02837
        options \rightarrow dialog = (GtkDialog *)
02838
          gtk_dialog_new_with_buttons (gettext ("Options"),
02839
                                         window->window.
02840
                                         GTK_DIALOG_MODAL,
                                         gettext ("_OK"), GTK_RESPONSE_OK,
gettext ("_Cancel"), GTK_RESPONSE_CANCEL,
02841
02842
02843
                                         NULL);
02844
        gtk_container add
02845
          (GTK_CONTAINER (gtk_dialog_get_content_area (options->dialog)),
02846
           GTK_WIDGET (options->grid));
02847
        if (gtk_dialog_run (options->dialog) == GTK_RESPONSE_OK)
02848
         {
02849
            input->seed
               = (unsigned long int) gtk_spin_button_get_value (options->spin_seed);
02850
02851
             nthreads = gtk_spin_button_get_value_as_int (options->spin_threads);
02852
            nthreads_gradient
02853
              = gtk_spin_button_get_value_as_int (options->spin_gradient);
02854
02855
        gtk_widget_destroy (GTK_WIDGET (options->dialog));
02856 }
02857
02862 void
02863 running_new ()
02864
02865 #if DEBUG
02866
       fprintf (stderr, "running_new: start\n");
02867 #endif
02868
       running->label = (GtkLabel *) gtk_label_new (gettext ("Calculating ..."));
02869
        running->dialog = (GtkDialog *)
02870
          gtk_dialog_new_with_buttons (gettext ("Calculating"),
02871
                                         window->window, GTK_DIALOG_MODAL, NULL, NULL);
02872
        gtk_container_add
        (GTK_CONTAINER (gtk_dialog_get_content_area (running->dialog)),
02873
02874
           GTK WIDGET (running->label));
02875
        gtk_widget_show_all (GTK_WIDGET (running->dialog));
02876 #if DEBUG
02877
       fprintf (stderr, "running_new: end\n");
02878 #endif
02879 }
02880
02886 int
02887 window_get_algorithm ()
02888 {
02889
       unsigned int i;
        for (i = 0; i < NALGORITHMS; ++i)
  if (gtk_toggle_button_get_active</pre>
02890
02891
              (GTK_TOGGLE_BUTTON (window->button_algorithm[i])))
02892
02893
            break;
02894
        return i;
02895 }
02896
02902 int
02903 window_get_gradient ()
02904 {
02905
        unsigned int i;
       for (i = 0; i < NGRADIENTS; ++i)
  if (gtk_toggle_button_get_active</pre>
02906
02907
02908
               (GTK_TOGGLE_BUTTON (window->button_gradient[i])))
02909
            break:
02910
        return i;
02911 }
02912
02917 void
02918 window_save_gradient ()
02919 {
02920 #if DEBUG
02921
        fprintf (stderr, "window_save_gradient: start\n");
02922 #endif
02923
        if (gtk_toggle_button_get_active (GTK_TOGGLE_BUTTON (window->check_gradient)))
02924
02925
            input->nsteps = gtk_spin_button_get_value_as_int (window->spin_steps);
             input->relaxation = gtk_spin_button_get_value (window->
02926
     spin_relaxation);
02927
            switch (window_get_gradient ())
02928
              case GRADIENT_METHOD_COORDINATES:
02929
                input->gradient_method = GRADIENT_METHOD_COORDINATES;
02930
02931
                break;
02932
              default:
02933
               input->gradient_method = GRADIENT_METHOD_RANDOM;
02934
                input->nestimates
02935
                   = gtk_spin_button_get_value_as_int (window->spin_estimates);
02936
              }
02937
          }
```

```
02938
       else
02939
         input->nsteps = 0;
02940 #if DEBUG
02941
       fprintf (stderr, "window_save_gradient: end\n");
02942 #endif
02943 }
02944
02950 int
02951 window_save ()
02952 {
02953
        char *buffer:
02954
        GtkFileChooserDialog *dlg;
02955
02956 #if DEBUG
02957
       fprintf (stderr, "window_save: start\n");
02958 #endif
02959
02960
        // Opening the saving dialog
        dlg = (GtkFileChooserDialog *)
02961
02962
          gtk_file_chooser_dialog_new (gettext ("Save file"),
02963
                                         window->window,
02964
                                        GTK_FILE_CHOOSER_ACTION_SAVE,
                                        gettext ("_Cancel"),
02965
02966
                                        GTK RESPONSE CANCEL.
                                        gettext ("_OK"), GTK_RESPONSE_OK, NULL);
02967
        gtk_file_chooser_set_do_overwrite_confirmation (GTK_FILE_CHOOSER (dlg), TRUE);
02968
02969
        buffer = g_build_filename (input->directory, input->name, NULL);
02970
        gtk_file_chooser_set_filename (GTK_FILE_CHOOSER (dlg), buffer);
        g_free (buffer);
02971
02972
02973
        // If OK response then saving
02974
        if (gtk_dialog_run (GTK_DIALOG (dlg)) == GTK_RESPONSE_OK)
02975
02976
02977
            // Adding properties to the root XML node
            input->simulator = gtk_file_chooser_get_filename
  (GTK_FILE_CHOOSER (window->button_simulator));
02978
02979
02980
            if (gtk_toggle_button_get_active
02981
                 (GTK_TOGGLE_BUTTON (window->check_evaluator)))
02982
              input->evaluator = gtk_file_chooser_get_filename
02983
                 (GTK_FILE_CHOOSER (window->button_evaluator));
02984
            else
02985
              input->evaluator = NULL:
02986
            input->result
02987
              = (char *) xmlStrdup ((const xmlChar *)
02988
                                     gtk_entry_get_text (window->entry_result));
            input->variables
02989
02990
              = (char *) xmlStrdup ((const xmlChar *)
                                     gtk_entry_get_text (window->entry_variables));
02991
02992
02993
            // Setting the algorithm
02994
            switch (window_get_algorithm ())
02995
02996
              case ALGORITHM_MONTE_CARLO:
                input->algorithm = ALGORITHM_MONTE_CARLO;
02997
02998
                input->nsimulations
02999
                   -
gtk_spin_button_get_value_as_int (window->spin_simulations);
03000
03001
                  = gtk_spin_button_get_value_as_int (window->spin_iterations);
03002
                input->tolerance = gtk_spin_button_get_value (window->
      spin tolerance);
03003
                input->nbest = gtk_spin_button_get_value_as_int (window->
     spin_bests);
03004
               window_save_gradient ();
03005
                break;
03006
              case ALGORITHM_SWEEP:
03007
                input->algorithm = ALGORITHM_SWEEP;
03008
                input->niterations
                  = gtk_spin_button_get_value_as_int (window->spin_iterations);
03009
03010
                input->tolerance = gtk_spin_button_get_value (window->
     spin_tolerance);
03011
                input->nbest = gtk_spin_button_get_value_as_int (window->
      spin_bests);
03012
                window_save_gradient ();
03013
                break;
03014
              default:
03015
                input->algorithm = ALGORITHM_GENETIC;
03016
                input->nsimulations
03017
                   = gtk_spin_button_get_value_as_int (window->spin_population);
03018
                input->niterations
03019
                  = gtk_spin_button_get_value_as_int (window->spin_generations);
03020
                input->mutation_ratio
03021
                    gtk_spin_button_get_value (window->spin_mutation);
03022
                input->reproduction_ratio
03023
                   = gtk_spin_button_get_value (window->spin_reproduction);
03024
                input->adaptation ratio
03025
                   = gtk_spin_button_get_value (window->spin_adaptation);
```

```
break;
03027
             }
03028
03029
            \ensuremath{//} Saving the XML file
           buffer = gtk_file_chooser_get_filename (GTK_FILE_CHOOSER (dlg));
03030
03031
           input save (buffer);
03033
            // Closing and freeing memory
03034
           g_free (buffer);
03035
            gtk_widget_destroy (GTK_WIDGET (dlg));
03036 #if DEBUG
           fprintf (stderr, "window_save: end\n");
03037
03038 #endif
03039
           return 1;
03040
03041
       // Closing and freeing memory
03042
03043
       gtk_widget_destroy (GTK_WIDGET (dlg));
03044 #if DEBUG
03045
       fprintf (stderr, "window_save: end\n");
03046 #endif
03047
       return 0;
03048 }
03049
03054 void
03055 window_run ()
03056 {
03057
       unsigned int i;
03058
       char *msg, *msg2, buffer[64], buffer2[64];
03059 #if DEBUG
03060
       fprintf (stderr, "window_run: start\n");
03061 #endif
03062 if (!window_save ())
03063
03064 #if DEBUG
           fprintf (stderr, "window_run: end\n");
03065
03066 #endif
03067
          return;
03068
03069
       running_new ();
03070
       while (gtk_events_pending ())
03071
         gtk_main_iteration ();
03072
       calibrate_open ();
       gtk_widget_destroy (GTK_WIDGET (running->dialog));
03073
03074
       snprintf (buffer, 64, "error = %.15le\n", calibrate->error_old[0]);
03075
        msg2 = g\_strdup (buffer);
03076
       for (i = 0; i < calibrate->nvariables; ++i, msg2 = msg)
03077
03078
           snprintf (buffer, 64, "%s = %s\n",
           calibrate->label[i], format[calibrate->precision[i]]);
snprintf (buffer2, 64, buffer, calibrate->value_old[i]);
03079
03080
03081
           msg = g_strconcat (msg2, buffer2, NULL);
           g_free (msg2);
03082
03083
       03084
03085
       msg = g_strconcat (msg2, buffer, NULL);
03086
03087
       g_free (msg2);
03088
       show_message (gettext ("Best result"), msg, INFO_TYPE);
03089
       g_free (msg);
       calibrate_free ();
03090
03091 #if DEBUG
03092
       fprintf (stderr, "window_run: end\n");
03093 #endif
03094 }
03095
03100 void
03101 window help ()
03102 {
03103
       char *buffer, *buffer2;
03104 buffer2 = g_build_filename (window->application_directory, "..", "manuals",
0.3105
                                    gettext ("user-manual.pdf"), NULL);
03106
       buffer = g_filename_to_uri (buffer2, NULL, NULL);
       g_free (buffer2);
03107
       gtk_show_uri (NULL, buffer, GDK_CURRENT_TIME, NULL);
03108
03109
       g_free (buffer);
03110 }
03111
03116 void
03117 window about ()
03118 {
03119
       static const gchar *authors[] = {
03120
          "Javier Burguete Tolosa <jburguete@eead.csic.es>",
03121
          "Borja Latorre Garcés <borja.latorre@csic.es>",
03122
         NULL
03123
03124
       gtk_show_about_dialog
```

```
(window->window,
            "program_name", "MPCOTool",
03126
03127
           "comments",
           gettext ("A software to perform calibrations/optimizations of empirical "
03128
                     "parameters"),
03129
           "authors", authors,
03130
           "translator-credits", "Javier Burguete Tolosa <jburguete@eead.csic.es>",
03131
           "version", "1.2.1",
"copyright", "Copyright 2012-2015 Javier Burguete Tolosa",
03132
03133
03134
           "logo", window->logo,
           "website", "https://github.com/jburguete/mpcotool", "license-type", GTK_LICENSE_BSD, NULL);
03135
03136
03137 }
03138
03144 void
03145 window_update_gradient ()
03146 {
03147
        gtk widget show (GTK WIDGET (window->check gradient));
03148
        if (gtk_toggle_button_get_active (GTK_TOGGLE_BUTTON (window->check_gradient)))
          gtk_widget_show (GTK_WIDGET (window->grid_gradient));
03149
03150
        switch (window_get_gradient ())
03151
03152
          case GRADIENT METHOD COORDINATES:
            gtk widget hide (GTK WIDGET (window->label estimates));
03153
            gtk_widget_hide (GTK_WIDGET (window->spin_estimates));
03154
03155
            break;
03156
03157
            gtk_widget_show (GTK_WIDGET (window->label_estimates));
            gtk_widget_show (GTK_WIDGET (window->spin_estimates));
03158
03159
03160 }
03161
03166 void
03167 window_update ()
03168 {
03169
        unsigned int i;
03170
        gtk_widget_set_sensitive
          (GTK_WIDGET (window->button_evaluator),
03171
03172
           gtk_toggle_button_get_active (GTK_TOGGLE_BUTTON
03173
                                           (window->check_evaluator)));
03174
        gtk_widget_hide (GTK_WIDGET (window->label_simulations));
        gtk_widget_hide (GTK_WIDGET (window->spin_simulations));
gtk_widget_hide (GTK_WIDGET (window->label_iterations));
03175
03176
03177
        gtk_widget_hide (GTK_WIDGET (window->spin_iterations));
        gtk_widget_hide (GTK_WIDGET (window->label_tolerance));
03178
03179
        gtk_widget_hide (GTK_WIDGET (window->spin_tolerance));
03180
        gtk_widget_hide (GTK_WIDGET (window->label_bests));
03181
        gtk_widget_hide (GTK_WIDGET (window->spin_bests));
        gtk_widget_hide (GTK_WIDGET (window->label_population));
03182
        gtk_widget_hide (GTK_WIDGET (window->spin_population));
03183
03184
        gtk_widget_hide (GTK_WIDGET (window->label_generations));
03185
        gtk_widget_hide (GTK_WIDGET (window->spin_generations));
03186
        gtk_widget_hide (GTK_WIDGET (window->label_mutation));
        gtk_widget_hide (GTK_WIDGET (window->spin_mutation));
gtk_widget_hide (GTK_WIDGET (window->label_reproduction));
03187
03188
        gtk_widget_hide (GTK_WIDGET (window->spin_reproduction));
03189
        gtk_widget_hide (GTK_WIDGET (window->label_adaptation));
03190
03191
        gtk_widget_hide (GTK_WIDGET (window->spin_adaptation));
03192
        gtk_widget_hide (GTK_WIDGET (window->label_sweeps));
03193
        gtk_widget_hide (GTK_WIDGET (window->spin_sweeps));
        gtk_widget_hide (GTK_WIDGET (window->label_bits));
03194
        gtk_widget_hide (GTK_WIDGET (window->spin_bits));
03195
03196
        gtk_widget_hide (GTK_WIDGET (window->check_gradient));
        gtk_widget_hide (GTK_WIDGET (window->grid_gradient));
03197
03198
        i = gtk_spin_button_get_value_as_int (window->spin_iterations);
03199
        switch (window_get_algorithm ())
03200
03201
          case ALGORITHM MONTE CARLO:
03202
            gtk_widget_show (GTK_WIDGET (window->label_simulations));
03203
            gtk_widget_show (GTK_WIDGET (window->spin_simulations));
03204
            gtk_widget_show (GTK_WIDGET (window->label_iterations));
03205
            gtk_widget_show (GTK_WIDGET (window->spin_iterations));
03206
            if (i > 1)
03207
03208
                gtk_widget_show (GTK_WIDGET (window->label_tolerance));
                gtk_widget_show (GTK_WIDGET (window->spin_tolerance));
03209
03210
                gtk_widget_show (GTK_WIDGET (window->label_bests));
03211
                gtk_widget_show (GTK_WIDGET (window->spin_bests));
03212
03213
            window_update_gradient ();
03214
            break;
          case ALGORITHM_SWEEP:
03215
03216
            gtk_widget_show (GTK_WIDGET (window->label_iterations));
03217
            gtk_widget_show (GTK_WIDGET (window->spin_iterations));
03218
            if (i > 1)
03219
03220
                qtk_widget_show (GTK_WIDGET (window->label_tolerance));
```

```
gtk_widget_show (GTK_WIDGET (window->spin_tolerance));
                gtk_widget_show (GTK_WIDGET (window->label_bests));
03222
03223
                gtk_widget_show (GTK_WIDGET (window->spin_bests));
03224
            gtk_widget_show (GTK_WIDGET (window->label_sweeps));
03225
03226
            gtk_widget_show (GTK_WIDGET (window->spin_sweeps));
            gtk_widget_show (GTK_WIDGET (window->check_gradient));
03228
            window_update_gradient ();
03229
            break;
03230
          default:
            gtk_widget_show (GTK_WIDGET (window->label_population));
03231
            gtk_widget_show (GTK_WIDGET (window->spin_population));
03232
03233
            gtk_widget_show (GTK_WIDGET (window->label_generations));
03234
            gtk_widget_show (GTK_WIDGET (window->spin_generations));
03235
            gtk_widget_show (GTK_WIDGET (window->label_mutation));
03236
            gtk_widget_show (GTK_WIDGET (window->spin_mutation));
            gtk_widget_show (GTK_WIDGET (window->label_reproduction));
03237
03238
            gtk_widget_show (GTK_WIDGET (window->spin_reproduction));
03239
            gtk_widget_show (GTK_WIDGET (window->label_adaptation));
03240
            gtk_widget_show (GTK_WIDGET (window->spin_adaptation));
03241
            gtk_widget_show (GTK_WIDGET (window->label_bits));
03242
            gtk_widget_show (GTK_WIDGET (window->spin_bits));
03243
03244
        {\tt gtk\_widget\_set\_sensitive}
03245
          (GTK_WIDGET (window->button_remove_experiment), input->
     nexperiments > 1);
03246
       gtk_widget_set_sensitive
03247
          (GTK_WIDGET (window->button_remove_variable), input->
     nvariables > 1);
03248
       for (i = 0; i < input->ninputs; ++i)
03249
03250
            gtk_widget_show (GTK_WIDGET (window->check_template[i]));
03251
            gtk_widget_show (GTK_WIDGET (window->button_template[i]));
03252
            gtk_widget_set_sensitive (GTK_WIDGET (window->check_template[i]), 0);
03253
            gtk_widget_set_sensitive (GTK_WIDGET (window->button_template[i]), 1);
03254
            g_signal_handler_block
03255
              (window->check template[i], window->id template[i]);
03256
            g_signal_handler_block (window->button_template[i], window->
     id_input[i]);
03257
           gtk_toggle_button_set_active
03258
              (GTK_TOGGLE_BUTTON (window->check_template[i]), 1);
03259
            g_signal_handler_unblock
03260
              (window->button template[i], window->id input[i]);
03261
            g_signal_handler_unblock
03262
              (window->check_template[i], window->id_template[i]);
03263
03264
        if (i > 0)
03265
            gtk_widget_set_sensitive (GTK_WIDGET (window->check_template[i - 1]), 1);
03266
03267
            atk widget set sensitive
03268
              (GTK_WIDGET (window->button_template[i - 1]),
               gtk_toggle_button_get_active
03269
03270
               GTK_TOGGLE_BUTTON (window->check_template[i - 1]));
03271
03272
        if (i < MAX NINPUTS)
03273
         {
           gtk_widget_show (GTK_WIDGET (window->check_template[i]));
            gtk_widget_show (GTK_WIDGET (window->button_template[i]));
03275
            gtk_widget_set_sensitive (GTK_WIDGET (window->check_template[i]), 1);
03276
03277
            gtk_widget_set_sensitive
03278
              (GTK WIDGET (window->button template[i]),
03279
               gtk_toggle_button_get_active
03280
               GTK_TOGGLE_BUTTON (window->check_template[i]));
03281
            g_signal_handler_block
03282
              (window->check_template[i], window->id_template[i]);
03283
            g_signal_handler_block (window->button_template[i], window->
     id_input[i]);
03284
            gtk toggle button set active
03285
             (GTK_TOGGLE_BUTTON (window->check_template[i]), 0);
03286
            g_signal_handler_unblock
              (window->button_template[i], window->id_input[i]);
03287
03288
            g_signal_handler_unblock
03289
              (window->check_template[i], window->id_template[i]);
03290
03291
        while (++i < MAX NINPUTS)
03292
            gtk_widget_hide (GTK_WIDGET (window->check_template[i]));
03293
03294
            gtk_widget_hide (GTK_WIDGET (window->button_template[i]));
03295
03296
        atk widget set sensitive
          (GTK WIDGET (window->spin minabs),
03297
03298
           gtk_toggle_button_get_active (GTK_TOGGLE_BUTTON (window->check_minabs)));
03299
        gtk_widget_set_sensitive
03300
          (GTK_WIDGET (window->spin_maxabs),
03301
           gtk_toggle_button_get_active (GTK_TOGGLE_BUTTON (window->check_maxabs)));
03302 }
03303
```

```
03308 void
03309 window_set_algorithm ()
03310 {
03311
        int i:
03312 #if DEBUG
03313
        fprintf (stderr, "window set algorithm: start\n");
03314 #endif
03315
       i = window_get_algorithm ();
03316
        switch (i)
03317
          case ALGORITHM SWEEP:
03318
03319
            input->nsweeps = (unsigned int *) g_realloc
03320
              (input->nsweeps, input->nvariables * sizeof (unsigned int));
03321
            i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03322
            <u>if</u> (i < 0)
03323
              i = 0:
03324
            gtk_spin_button_set_value (window->spin_sweeps,
03325
                                         (qdouble) input->nsweeps[i]);
03326
           break;
          case ALGORITHM_GENETIC:
03327
03328
           input->nbits = (unsigned int *) g_realloc
03329
              (input->nbits, input->nvariables * sizeof (unsigned int));
            \label{eq:combo_box_get_active} \verb| i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable)); \\
03330
            if (i < 0)
03331
              i = 0;
03332
03333
            gtk_spin_button_set_value (window->spin_bits, (gdouble) input->
     nbits[i]);
03334
03335
        window_update ();
03336 #if DEBUG
03337 fprintf (stderr, "window_set_algorithm: end\n");
03338 #endif
03339 }
03340
03345 void
03346 window_set_experiment ()
03347 {
03348
       unsigned int i, j;
03349
        char *buffer1, *buffer2;
03350 #if DEBUG
03351
       fprintf (stderr, "window_set_experiment: start\n");
03352 #endif
       i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_experiment));
03353
03354
        gtk_spin_button_set_value (window->spin_weight, input->weight[i]);
        buffer1 = gtk_combo_box_text_get_active_text (window->combo_experiment);
03355
03356
        buffer2 = g_build_filename (input->directory, buffer1, NULL);
03357
        g_free (buffer1);
        g_signal_handler_block
03358
          (window->button_experiment, window->id_experiment name);
03359
03360
        gtk_file_chooser_set_filename
03361
          (GTK_FILE_CHOOSER (window->button_experiment), buffer2);
03362
        g_signal_handler_unblock
03363
          (window->button_experiment, window->id_experiment_name);
03364
        g_free (buffer2);
        for (j = 0; j < input->ninputs; ++j)
03365
03366
03367
            g_signal_handler_block (window->button_template[j], window->
      id_input[j]);
03368
           buffer2
03369
              = g_build_filename (input->directory, input->template[j][i], NULL);
03370
            {\tt gtk\_file\_chooser\_set\_filename}
              (GTK_FILE_CHOOSER (window->button_template[j]), buffer2);
03371
03372
            g_free (buffer2);
03373
            g_signal_handler_unblock
03374
              (window->button_template[j], window->id_input[j]);
03375
03376 #if DEBUG
03377
        fprintf (stderr, "window set experiment: end\n");
03378 #endif
03379 }
03380
03385 void
03386 window_remove_experiment ()
03387 {
03388
        unsigned int i, j;
       i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_experiment));
03389
        g_signal_handler_block (window->combo_experiment, window->
03390
03391
        gtk_combo_box_text_remove (window->combo_experiment, i);
g_signal_handler_unblock (window->combo_experiment, window->
03392
      id experiment);
03393
        xmlFree (input->experiment[i]);
03394
         --input->nexperiments;
        for (j = i; j < input->nexperiments; ++j)
03395
03396
            input->experiment[j] = input->experiment[j + 1];
03397
03398
            input->weight[i] = input->weight[i + 1];
```

```
j = input->nexperiments - 1;
03400
03401
        if (i > j)
03402
         i = j;
        for (j = 0; j < input->ninputs; ++j)
03403
          g_signal_handler_block (window->button_template[j], window->
03404
     id_input[j]);
03405
        g_signal_handler_block
03406
          (window->button_experiment, window->id_experiment_name);
03407
        gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_experiment), i);
03408
        {\tt g\_signal\_handler\_unblock}
03409
          (window->button experiment, window->id experiment name);
03410
        for (j = 0; j < input->ninputs; ++j)
         g_signal_handler_unblock (window->button_template[j], window->
     id_input[j]);
03412
       window_update ();
03413 }
03414
03419 void
03420 window_add_experiment ()
03421 {
03422
        unsigned int i, j;
       i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_experiment));
03423
03424
        g_signal_handler_block (window->combo_experiment, window->
     id_experiment);
03425 gtk_combo_box_text_insert_text
03426
          (window->combo_experiment, i, input->experiment[i]);
03427
        g_signal_handler_unblock (window->combo_experiment, window->
     id_experiment);
03428
        input->experiment = (char **) g_realloc
03429
          (input->experiment, (input->nexperiments + 1) * sizeof (char *));
03430
        input->weight = (double *) g_realloc
03431
          (input->weight, (input->nexperiments + 1) * sizeof (double));
03432
        for (j = input->nexperiments - 1; j > i; --j)
03433
            input->experiment[j + 1] = input->experiment[j];
input->weight[j + 1] = input->weight[j];
03434
03435
03436
03437
        input->experiment[j + 1]
03438
          = (char *) xmlStrdup ((xmlChar *) input->experiment[j]);
03439
        input->weight[j + 1] = input->weight[j];
03440
        ++input->nexperiments;
        for (j = 0; j < input->ninputs; ++j)
03441
03442
          g_signal_handler_block (window->button_template[j], window->
      id_input[j]);
03443
        g_signal_handler_block
03444
          (window->button_experiment, window->id_experiment_name);
03445
        gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_experiment), i + 1);
        g_signal_handler_unblock
03446
03447
          (window->button experiment, window->id experiment name);
        for (j = 0; j < input->ninputs; ++j)
03448
          g_signal_handler_unblock (window->button_template[j], window->
03449
     id_input[j]);
03450
       window_update ();
03451 }
03452
03458 window_name_experiment ()
03459 {
03460
       unsigned int i;
       char *buffer;
GFile *file1, *file2;
0.3461
03462
03463 #if DEBUG
03464
       fprintf (stderr, "window_name_experiment: start\n");
03465 #endif
03466
        i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_experiment));
03467
        file1
          = gtk file chooser get file (GTK FILE CHOOSER (window->button experiment));
03468
03469
        file2 = g_file_new_for_path (input->directory);
        buffer = g_file_get_relative_path (file2, file1);
        g_signal_handler_block (window->combo_experiment, window->
03471
      id experiment);
03472
        gtk_combo_box_text_remove (window->combo_experiment, i);
03473
        qtk_combo_box_text_insert_text (window->combo_experiment, i, buffer);
        gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_experiment), i);
03474
        g_signal_handler_unblock (window->combo_experiment, window->
     id_experiment);
03476 g_free (buffer);
       g_object_unref (file2);
g_object_unref (file1);
03477
03478
03479 #if DEBUG
03480
       fprintf (stderr, "window_name_experiment: end\n");
03481 #endif
03482 }
03483
03488 void
03489 window weight experiment ()
```

```
03490 {
03491
        unsigned int i;
03492 #if DEBUG
       fprintf (stderr, "window_weight_experiment: start\n");
03493
03494 #endif
       i = qtk_combo_box_qet_active (GTK_COMBO_BOX (window->combo_experiment));
03495
       input->weight[i] = gtk_spin_button_get_value (window->spin_weight);
03497 #if DEBUG
03498
       fprintf (stderr, "window_weight_experiment: end\n");
03499 #endif
03500 }
03501
03507 void
03508 window_inputs_experiment ()
03509 {
03510
        unsigned int j;
03511 #if DEBUG
        fprintf (stderr, "window inputs experiment: start\n");
03512
03513 #endif
03514
        j = input->ninputs - 1;
03515
03516
             && !gtk_toggle_button_get_active (GTK_TOGGLE_BUTTON
03517
                                                 (window->check_template[j])))
03518
        --input->ninputs;
if (input->ninputs < MAX_NINPUTS</pre>
03519
03520
             && gtk_toggle_button_get_active (GTK_TOGGLE_BUTTON
03521
                                                 (window->check_template[j])))
03522
03523
             ++input->ninputs;
03524
             for (j = 0; j < input->ninputs; ++j)
03525
03526
                input->template[j] = (char **)
03527
                   g_realloc (input->template[j], input->nvariables * sizeof (char *));
03528
              }
03529
        window_update ();
03530
03531 #if DEBUG
03532 fprintf (stderr, "window_inputs_experiment: end\n");
03533 #endif
03534 }
03535
03543 void
03544 window template experiment (void *data)
03545 {
03546
       unsigned int i, j;
03547
        char *buffer;
03548 GFile *file1, *file2;
03549 #if DEBUG
       fprintf (stderr, "window template experiment: start\n");
03550
03551 #endif
       i = (size_t) data;
03553
         j = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_experiment));
        fileĺ
03554
03555
          = gtk_file_chooser_get_file (GTK_FILE_CHOOSER (window->button_template[i]));
       file2 = g_file_new_for_path (input->directory);
buffer = g_file_get_relative_path (file2, file1);
input->template[i][j] = (char *) xmlStrdup ((xmlChar *) buffer);
03556
03557
03558
03559
        g_free (buffer);
        g_object_unref (file2);
g_object_unref (file1);
03560
03561
03562 #if DEBUG
03563 fprintf (stderr, "window_template_experiment: end\n");
03564 #endif
03565 }
03566
03571 void
03572 window_set_variable ()
03573 {
03574
        unsigned int i:
03575 #if DEBUG
03576
        fprintf (stderr, "window_set_variable: start\n");
03577 #endif
03578 i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03579
        g_signal_handler_block (window->entry_variable, window->
      id variable label);
03580 gtk_entry_set_text (window->entry_variable, input->label[i]);
03581
        g_signal_handler_unblock (window->entry_variable, window->
      id_variable_label);
03582
        gtk_spin_button_set_value (window->spin_min, input->rangemin[i]);
        gtk_spin_button_set_value (window->spin_max, input->rangemax[i]);
if (input->rangeminabs[i] != -G_MAXDOUBLE)
03583
03584
03585
          {
            gtk_spin_button_set_value (window->spin_minabs, input->
      rangeminabs[i]);
03587
            gtk_toggle_button_set_active
               (GTK_TOGGLE_BUTTON (window->check_minabs), 1);
03588
03589
```

```
else
03591
03592
            gtk_spin_button_set_value (window->spin_minabs, -G_MAXDOUBLE);
03593
            gtk_toggle_button_set_active
              (GTK TOGGLE BUTTON (window->check minabs), 0);
03594
03595
03596
        if (input->rangemaxabs[i] != G_MAXDOUBLE)
03597
         {
03598
            gtk_spin_button_set_value (window->spin_maxabs, input->
     rangemaxabs[i]);
03599
            gtk_toggle_button_set_active
              (GTK_TOGGLE_BUTTON (window->check_maxabs), 1);
03600
03601
03602
        else
03603
03604
            gtk_spin_button_set_value (window->spin_maxabs, G_MAXDOUBLE);
03605
            gtk_toggle_button_set_active
               (GTK_TOGGLE_BUTTON (window->check_maxabs), 0);
03606
03607
03608
       gtk_spin_button_set_value (window->spin_precision, input->
      precision[i]);
03609 #if DEBUG
        fprintf (stderr, "window_set_variable: precision[%u]=%u\n", i,
03610
03611
                 input->precision[i]);
03612 #endif
03613
       switch (window_get_algorithm ())
03614
          case ALGORITHM_SWEEP:
03615
03616
            gtk_spin_button_set_value (window->spin_sweeps,
03617
                                         (gdouble) input->nsweeps[i]);
03618 #if DEBUG
03619
           fprintf (stderr, "window_set_variable: nsweeps[%u]=%u\n", i,
03620
                     input->nsweeps[i]);
03621 #endif
            break;
03622
          case ALGORITHM_GENETIC:
03623
            gtk_spin_button_set_value (window->spin_bits, (gdouble) input->
03624
     nbits[i]);
03625 #if DEBUG
03626
          fprintf (stderr, "window_set_variable: nbits[%u]=%u\n", i,
03627
                      input->nbits[i]);
03628 #endif
03629
           break:
03630
        window_update ();
03632 #if DEBUG
03633 fprintf (stderr, "window_set_variable: end\n");
03634 #endif
03635 }
03636
03641 void
03642 window_remove_variable ()
03643 {
03644
        unsigned int i, j;
        i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03645
        g_signal_handler_block (window->combo_variable, window->
03646
     id_variable);
03647
       gtk_combo_box_text_remove (window->combo_variable, i);
        g_signal_handler_unblock (window->combo_variable, window->
03648
     id_variable);
03649
        xmlFree (input->label[i]);
03650
        --input->nvariables;
03651
        for (j = i; j < input->nvariables; ++j)
03652
03653
            input->label[j] = input->label[j + 1];
            input->rangemin[j] = input->rangemin[j + 1];
input->rangemax[j] = input->rangemax[j + 1];
03654
03655
            input->rangeminabs[j] = input->rangeminabs[j + 1];
input->rangemaxabs[j] = input->rangemaxabs[j + 1];
03656
03657
            input->precision[j] = input->precision[j + 1];
switch (window_get_algorithm ())
03658
03659
03660
              {
03661
              case ALGORITHM_SWEEP:
                input->nsweeps[j] = input->nsweeps[j + 1];
03662
03663
                break;
03664
              case ALGORITHM_GENETIC:
03665
                input->nbits[j] = input->nbits[j + 1];
03666
03667
03668
        j = input->nvariables - 1;
        if (i > j)
i = j;
03669
03670
        g_signal_handler_block (window->entry_variable, window->
     id_variable_label);
03672 gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_variable), i);
03673
        g_signal_handler_unblock (window->entry_variable, window->
      id_variable_label);
```

```
window_update ();
03675 }
03676
03681 void
03682 window add variable ()
03683 {
03684
         unsigned int i, j;
03685 #if DEBUG
03686
         fprintf (stderr, "window_add_variable: start\n");
03687 #endif
         i = qtk_combo_box_qet_active (GTK_COMBO_BOX (window->combo_variable));
03688
03689
         g_signal_handler_block (window->combo_variable, window->
      id_variable);
         qtk_combo_box_text_insert_text (window->combo_variable, i, input->
      label[i]);
03691
         g_signal_handler_unblock (window->combo_variable, window->
       id variable);
03692
         input->label = (char **) g realloc
            (input->label, (input->nvariables + 1) * sizeof (char *));
03693
         input->rangemin = (double *) g_realloc
03694
03695
            (input->rangemin, (input->nvariables + 1) * sizeof (double));
03696
         input->rangemax = (double *) g_realloc
         (input->rangemax, (input->nvariables + 1) * sizeof (double));
input->rangeminabs = (double *) g_realloc
03697
03698
03699
            (input->rangeminabs, (input->nvariables + 1) * sizeof (double));
03700
          input->rangemaxabs = (double *) g_realloc
03701
            (input->rangemaxabs, (input->nvariables + 1) * sizeof (double));
03702
         input->precision = (unsigned int *) g_realloc
          (input->precision, (input->nvariables + 1) * sizeof (unsigned int));
for (j = input->nvariables - 1; j > i; --j)
03703
03704
03705
03706
              input->label[j + 1] = input->label[j];
              input->rangemin[j + 1] = input->rangemin[j];
input->rangemax[j + 1] = input->rangemax[j];
03707
03708
              input->rangeminabs[j + 1] = input->rangeminabs[j];
input->rangemaxabs[j + 1] = input->rangemaxabs[j];
03709
03710
03711
              input->precision[j + 1] = input->precision[j];
03712
03713
          input->label[j + 1] = (char *) xmlStrdup ((xmlChar *) input->label[j]);
         input->rangemin[j + 1] = input->rangemin[j];
input->rangemax[j + 1] = input->rangemax[j];
03714
03715
         input->rangeminabs[j + 1] = input->rangeminabs[j];
input->rangemaxabs[j + 1] = input->rangemaxabs[j];
input->precision[j + 1] = input->precision[j];
03716
03717
03718
03719
         switch (window_get_algorithm ())
03720
03721
            case ALGORITHM SWEEP:
03722
              input->nsweeps = (unsigned int *) g_realloc
              (input->nsweeps, (input->nvariables + 1) * sizeof (unsigned int));
for (j = input->nvariables - 1; j > i; --j)
03723
03724
                input->nsweeps[j + 1] = input->nsweeps[j];
03725
03726
              input->nsweeps[j + 1] = input->nsweeps[j];
03727
              break;
03728
            case ALGORITHM_GENETIC:
              input->nbits = (unsigned int *) g_realloc
03729
              (input->nbits (input->nvariables + 1) * sizeof (unsigned int));
for (j = input->nvariables - 1; j > i; --j)
03730
03731
03732
                input->nbits[j + 1] = input->nbits[j];
03733
              input->nbits[j + 1] = input->nbits[j];
03734
03735
         ++input->nvariables:
         g_signal_handler_block (window->entry_variable, window->
03736
      id_variable_label);
03737 gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_variable), i + 1);
03738 g_signal_handler_unblock (window->entry_variable, window->
      id_variable_label);
03739
         window_update ();
03740 #if DEBUG
03741
         fprintf (stderr, "window_add_variable: end\n");
03742 #endif
03743 }
03744
03749 void
03750 window label variable ()
03751 {
03752
         unsigned int i;
03753
         const char *buffer;
03754 #if DEBUG
         fprintf (stderr, "window_label_variable: start\n");
03755
03756 #endif
        i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03757
         buffer = gtk_entry_get_text (window->entry_variable);
03758
         g_signal_handler_block (window->combo_variable, window->
      id_variable);
03760
        gtk_combo_box_text_remove (window->combo_variable, i);
         gtk_combo_box_text_insert_text (window->combo_variable, i, buffer);
gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_variable), i);
03761
03762
```

```
03763
        g_signal_handler_unblock (window->combo_variable, window->
      id_variable);
03764 #if DEBUG
       fprintf (stderr, "window_label_variable: end\n");
03765
03766 #endif
03767 }
03768
03773 void
03774 window_precision_variable ()
03775 {
03776
        unsigned int i;
03777 #if DEBUG
03778
        fprintf (stderr, "window_precision_variable: start\n");
03779 #endif
03780
        i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03781
        input->precision[i]
03782
          = (unsigned int) gtk_spin_button_get_value_as_int (window->spin_precision);
03783
        gtk_spin_button_set_digits (window->spin_min, input->precision[i]);
gtk_spin_button_set_digits (window->spin_max, input->precision[i]);
03784
03785
        gtk_spin_button_set_digits (window->spin_minabs, input->precision[i]);
03786
        gtk_spin_button_set_digits (window->spin_maxabs, input->precision[i]);
03787 #if DEBUG
03788
        fprintf (stderr, "window_precision_variable: end\n");
03789 #endif
03790 }
03791
03796 void
03797 window_rangemin_variable ()
03798 {
03799
        unsigned int i:
03800 #if DEBUG
03801
        fprintf (stderr, "window_rangemin_variable: start\n");
03802 #endif
03803 i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03804
        input->rangemin[i] = gtk_spin_button_get_value (window->spin_min);
03805 #if DEBUG
03806
        fprintf (stderr, "window rangemin variable: end\n");
03807 #endif
03808 }
03809
03814 void
03815 window_rangemax_variable ()
03816 {
03817
        unsigned int i;
03818 #if DEBUG
03819
        fprintf (stderr, "window_rangemax_variable: start\n");
03820 #endif
03821 i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03822
        input->rangemax[i] = gtk_spin_button_get_value (window->spin_max);
03823 #if DEBUG
03824
        fprintf (stderr, "window_rangemax_variable: end\n");
03825 #endif
03826 }
03827
03832 void
03833 window rangeminabs variable ()
03834 {
03835
        unsigned int i;
03836 #if DEBUG
03837
        fprintf (stderr, "window_rangeminabs_variable: start\n");
03838 #endif
03839 i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03840
        input->rangeminabs[i] = gtk_spin_button_get_value (window->
      spin_minabs);
03841 #if DEBUG
03842
        fprintf (stderr, "window_rangeminabs_variable: end\n");
03843 #endif
03844 }
03845
03850 void
03851 window_rangemaxabs_variable ()
03852 {
03853
        unsigned int i;
03854 #if DEBUG
        fprintf (stderr, "window_rangemaxabs_variable: start\n");
03855
03856 #endif
03857 i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03858 input->rangemaxabs[i] = gtk_spin_button_get_value (window->
      spin_maxabs);
03859 #if DEBUG
03860 fprintf (stderr, "window_rangemaxabs_variable: end\n");
03861 #endif
03862 }
03863
03868 void
03869 window_update_variable ()
03870 {
```

```
03871
        int i;
03872 #if DEBUG
03873
        fprintf (stderr, "window_update_variable: start\n");
03874 #endif
       i = gtk_combo_box_get_active (GTK_COMBO_BOX (window->combo_variable));
03875
03876
        <u>if</u> (i < 0)
         i = 0;
03877
03878
        switch (window_get_algorithm ())
03879
03880
          case ALGORITHM SWEEP:
03881
03882 = gtk_spin_button_get_value_as_int (window->spin_sweeps);
03883 #if DEBUG
03884
           fprintf (stderr, "window_update_variable: nsweeps[%d]=%u\n", i,
03885
                      input->nsweeps[i]);
03886 #endif
03887
            break:
          case ALGORITHM_GENETIC:
03888
03889
            input->nbits[i] = gtk_spin_button_get_value_as_int (window->spin_bits);
03890 #if DEBUG
03891
           fprintf (stderr, "window_update_variable: nbits[%d]=%u\n", i,
03892
                      input->nbits[i]);
03893 #endif
03894
03895 #if DEBUG
       fprintf (stderr, "window_update_variable: end\n");
03897 #endif
03898 }
03899
03907 int
03908 window_read (char *filename)
03909 {
03910
       unsigned int i;
0.3911
        char *buffer;
03912 #if DEBUG
       fprintf (stderr, "window_read: start\n");
03913
03914 #endif
03915
03916
        // Reading new input file
03917
       input_free ();
03918
       if (!input_open (filename))
03919
         return 0;
03920
03921
        // Setting GTK+ widgets data
03922
       gtk_entry_set_text (window->entry_result, input->result);
03923
        gtk_entry_set_text (window->entry_variables, input->variables);
03924
       buffer = g_build_filename (input->directory, input->simulator, NULL);
03925
        {\tt gtk\_file\_chooser\_set\_filename} \ \ ({\tt GTK\_FILE\_CHOOSER}
03926
                                        (window->button simulator), buffer);
03927
        g free (buffer):
03928
        gtk_toggle_button_set_active (GTK_TOGGLE_BUTTON (window->check_evaluator),
03929
                                       (size_t) input->evaluator);
        if (input->evaluator)
03930
03931
            buffer = g_build_filename (input->directory, input->evaluator, NULL);
03932
03933
            gtk_file_chooser_set_filename (GTK_FILE_CHOOSER
03934
                                            (window->button_evaluator), buffer);
03935
            g_free (buffer);
03936
03937
        gtk_toggle_button_set_active
          (GTK_TOGGLE_BUTTON (window->button_algorithm[input->
03938
     algorithm]), TRUE);
03939
        switch (input->algorithm)
03940
03941
          case ALGORITHM_MONTE_CARLO:
03942
            gtk_spin_button_set_value (window->spin_simulations,
03943
                                        (gdouble) input->nsimulations);
03944
          case ALGORITHM SWEEP:
03945
            gtk_spin_button_set_value (window->spin_iterations,
                                        (gdouble) input->niterations);
03946
03947
            gtk_spin_button_set_value (window->spin_bests, (gdouble) input->
     nbest);
03948
            gtk_spin_button_set_value (window->spin_tolerance, input->
     tolerance);
03949
            gtk_toggle_button_set_active (GTK_TOGGLE_BUTTON (window->check_gradient),
03950
                                           input->nsteps);
03951
            if (input->nsteps)
03952
03953
                {\tt gtk\_toggle\_button\_set\_active}
                   (GTK_TOGGLE_BUTTON (window->button_gradient
03954
                                       [input->gradient_method]), TRUE);
03955
03956
                gtk_spin_button_set_value (window->spin_steps,
03957
                                             (gdouble) input->nsteps);
03958
                gtk_spin_button_set_value (window->spin_relaxation,
03959
                                             (gdouble) input->relaxation);
                switch (input->gradient_method)
03960
03961
```

```
case GRADIENT_METHOD_RANDOM:
03963
                   gtk_spin_button_set_value (window->spin_estimates,
03964
                                               (gdouble) input->nestimates);
03965
                 }
03966
             }
           break;
03967
03968
         default:
03969
           gtk_spin_button_set_value (window->spin_population,
03970
                                       (gdouble) input->nsimulations);
03971
            gtk_spin_button_set_value (window->spin_generations,
                                       (gdouble) input->niterations);
03972
03973
            gtk_spin_button_set_value (window->spin_mutation, input->
     mutation_ratio);
03974
           gtk_spin_button_set_value (window->spin_reproduction,
03975
                                       input->reproduction_ratio);
03976
            gtk_spin_button_set_value (window->spin_adaptation,
03977
                                       input->adaptation_ratio);
03978
03979
       g_signal_handler_block (window->combo_experiment, window->
     id_experiment);
       g_signal_handler_block (window->button_experiment,
03980
03981
                                window->id_experiment_name);
03982
       gtk_combo_box_text_remove_all (window->combo_experiment);
03983
       for (i = 0; i < input->nexperiments; ++i)
03984
         gtk_combo_box_text_append_text (window->combo_experiment,
                                         input->experiment[i]);
03985
03986
       {\tt g\_signal\_handler\_unblock}
03987
          (window->button_experiment, window->id_experiment_name);
03988
        g_signal_handler_unblock (window->combo_experiment, window->
     id_experiment);
03989
       gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_experiment), 0);
03990
        g_signal_handler_block (window->combo_variable, window->
      id_variable);
03991
        g_signal_handler_block (window->entry_variable, window->
     id_variable_label);
03992
       gtk_combo_box_text_remove_all (window->combo_variable);
        for (i = 0; i < input->nvariables; ++i)
03993
03994
         gtk_combo_box_text_append_text (window->combo_variable, input->
     label[i]);
03995
       g_signal_handler_unblock (window->entry_variable, window->
     id_variable_label);
03996
       g_signal_handler_unblock (window->combo_variable, window->
     id_variable);
03997
       gtk_combo_box_set_active (GTK_COMBO_BOX (window->combo_variable), 0);
       window_set_variable ();
03998
03999
       window_update ();
04000
04001 #if DEBUG
04002
       fprintf (stderr, "window_read: end\n");
04003 #endif
04004
       return 1;
04005 }
04006
04011 void
04012 window_open ()
04013 {
04014
       char *buffer, *directory, *name;
04015
       GtkFileChooserDialog *dlg;
04016
04017 #if DEBUG
       fprintf (stderr, "window_open: start\n");
04018
04019 #endif
04020
04021
        // Saving a backup of the current input file
04022
       directory = g_strdup (input->directory);
04023
       name = g_strdup (input->name);
04024
04025
        // Opening dialog
04026
       dlg = (GtkFileChooserDialog *)
04027
         gtk_file_chooser_dialog_new (gettext ("Open input file"),
04028
                                       window->window,
04029
                                       GTK_FILE_CHOOSER_ACTION_OPEN,
       04030
04031
04032
04033
04034
04035
            // Traying to open the input file
04036
           buffer = gtk_file_chooser_get_filename (GTK_FILE_CHOOSER (dlg));
04037
           if (!window read (buffer))
04038
04039 #if DEBUG
04040
               fprintf (stderr, "window_open: error reading input file\n");
04041 #endif
04042
               g_free (buffer);
04043
04044
               // Reading backup file on error
```

```
buffer = g_build_filename (directory, name, NULL);
04046
                if (!input_open (buffer))
04047
04048
04049
                   // Closing on backup file reading error
04050 #if DEBUG
04051
                   fprintf (stderr, "window_read: error reading backup file\n");
04052 #endif
                  g_free (buffer);
04053
04054
                   break;
             g_free (buffer);
}
04055
04056
04057
           else
04058
04059
             {
04060
               g_free (buffer);
04061
               break:
             }
04062
04063
         }
04064
04065
       // Freeing and closing
04066
       g_free (name);
04067
       g_free (directory);
       gtk_widget_destroy (GTK_WIDGET (dlg));
04068
04069 #if DEBUG
04070
       fprintf (stderr, "window_open: end\n");
04071 #endif
04072 }
04073
04078 void
04079 window_new ()
04080 {
04081
       unsigned int i;
04082
       char *buffer, *buffer2, buffer3[64];
04083
       GtkViewport *viewport;
       char *label_algorithm[NALGORITHMS] = {
04084
          "_Monte-Carlo", gettext ("_Sweep"), gettext ("_Genetic")
04085
04086
04087
       char *tip_algorithm[NALGORITHMS] = {
        gettext ("Monte-Carlo brute force algorithm"),
gettext ("Sweep brute force algorithm"),
04088
04089
         gettext ("Genetic algorithm")
04090
04091
04092
       char *label_gradient[NGRADIENTS] = {
04093
         gettext ("_Coordinates descent"), gettext ("_Random")
04094
04095
       char *tip_gradient[NGRADIENTS] = {
04096
         gettext ("Coordinates descent gradient estimate method"),
         gettext ("Random gradient estimate method")
04097
04098
04099
04100
        // Creating the window
04101
       window->window = (GtkWindow *) gtk_window_new (GTK_WINDOW_TOPLEVEL);
04102
       // Finish when closing the window
04103
       g_signal_connect (window->window, "delete-event", gtk_main_quit, NULL);
04104
04105
04106
        // Setting the window title
04107
       gtk_window_set_title (window->window, PROGRAM_INTERFACE);
04108
04109
       // Creating the open button
       window->button_open = (GtkToolButton *) gtk_tool_button_new
04110
04111
          (gtk_image_new_from_icon_name ("document-open",
04112
                                        GTK_ICON_SIZE_LARGE_TOOLBAR),
04113
           gettext ("Open"));
04114
       g_signal_connect (window->button_open, "clicked", window_open, NULL);
04115
04116
        // Creating the save button
       window->button_save = (GtkToolButton *) gtk_tool_button_new
04117
         (gtk_image_new_from_icon_name ("document-save",
04118
04119
                                        GTK_ICON_SIZE_LARGE_TOOLBAR),
           gettext ("Save"));
04120
04121
       g_signal_connect (window->button_save, "clicked", (void (*))
     window_save,
04122
                          NULL);
04123
04124
        // Creating the run button
04125
       window->button_run = (GtkToolButton *) gtk_tool_button_new
04126
          (gtk_image_new_from_icon_name ("system-run",
                                        GTK_ICON_SIZE_LARGE_TOOLBAR),
04127
04128
           gettext ("Run"));
04129
       g_signal_connect (window->button_run, "clicked", window_run, NULL);
04130
04131
        // Creating the options button
04132
        window->button_options = (GtkToolButton *) gtk_tool_button_new
          04133
04134
```

```
04135
           gettext ("Options"));
        g_signal_connect (window->button_options, "clicked", options_new, NULL);
04136
04137
04138
        // Creating the help button
        window->button_help = (GtkToolButton *) gtk_tool_button_new
04139
          (gtk_image_new_from_icon_name ("help-browser"
04140
04141
                                           GTK_ICON_SIZE_LARGE_TOOLBAR),
04142
           gettext ("Help"));
04143
        g_signal_connect (window->button_help, "clicked", window_help, NULL);
04144
04145
        // Creating the about button
        window->button_about = (GtkToolButton *) gtk_tool_button_new
04146
          (gtk_image_new_from_icon_name ("help-about",
04147
04148
                                           GTK_ICON_SIZE_LARGE_TOOLBAR),
04149
            gettext ("About"));
04150
        g_signal_connect (window->button_about, "clicked", window_about, NULL);
04151
04152
        // Creating the exit button
04153
        window->button_exit = (GtkToolButton *) gtk_tool_button_new
04154
          (gtk_image_new_from_icon_name ("application-exit"
04155
                                          GTK_ICON_SIZE_LARGE_TOOLBAR),
04156
            gettext ("Exit"));
04157
        g_signal_connect (window->button_exit, "clicked", gtk_main_quit, NULL);
04158
04159
        // Creating the buttons bar
04160
        window->bar_buttons = (GtkToolbar *) gtk_toolbar_new ();
04161
        gtk_toolbar_insert
04162
           (window->bar_buttons, GTK_TOOL_ITEM (window->button_open), 0);
04163
        gtk_toolbar_insert
04164
          (window->bar_buttons, GTK_TOOL_ITEM (window->button_save), 1);
04165
        gtk_toolbar_insert
04166
          (window->bar_buttons, GTK_TOOL_ITEM (window->button_run), 2);
04167
        gtk_toolbar_insert
04168
          (window->bar_buttons, GTK_TOOL_ITEM (window->button_options), 3);
04169
        gtk_toolbar_insert
04170
          (window->bar_buttons, GTK_TOOL_ITEM (window->button_help), 4);
04171
        gtk toolbar insert
04172
          (window->bar_buttons, GTK_TOOL_ITEM (window->button_about), 5);
04173
        gtk_toolbar_insert
04174
           (window->bar_buttons, GTK_TOOL_ITEM (window->button_exit), 6);
04175
        gtk_toolbar_set_style (window->bar_buttons, GTK_TOOLBAR_BOTH);
04176
04177
        // Creating the simulator program label and entry
04178
        window->label_simulator
04179
          = (GtkLabel *) gtk_label_new (gettext ("Simulator program"));
04180
        window->button_simulator = (GtkFileChooserButton *)
04181
          gtk_file_chooser_button_new (gettext ("Simulator program"),
        GTK_FILE_CHOOSER_ACTION_OPEN);
gtk_widget_set_tooltip_text (GTK_WIDGET (window->button_simulator),
04182
04183
                                       gettext ("Simulator program executable file"));
04184
04185
        // Creating the evaluator program label and entry
window->check_evaluator = (GtkCheckButton *)
04186
04187
          gtk_check_button_new_with_mnemonic (gettext ("_Evaluator program"));
04188
04189
        g_signal_connect (window->check_evaluator, "toggled",
      window_update, NULL);
04190
       window->button_evaluator = (GtkFileChooserButton *)
04191
          gtk_file_chooser_button_new (gettext ("Evaluator program"),
04192
                                         GTK_FILE_CHOOSER_ACTION_OPEN);
04193
        {\tt gtk\_widget\_set\_tooltip\_text}
04194
          (GTK WIDGET (window->button evaluator),
04195
           gettext ("Optional evaluator program executable file"));
04196
04197
        \ensuremath{//} Creating the results files labels and entries
        window->label_result = (GtkLabel *) gtk_label_new (gettext ("Result file"));
window->entry_result = (GtkEntry *) gtk_entry_new ();
04198
04199
04200
        {\tt gtk\_widget\_set\_tooltip\_text}
04201
          (GTK_WIDGET (window->entry_result), gettext ("Best results file"));
04202
        window->label_variables
04203
            (GtkLabel *) gtk_label_new (gettext ("Variables file"));
04204
        window->entry_variables = (GtkEntry *) gtk_entry_new ();
04205
        gtk_widget_set_tooltip_text
04206
          (GTK_WIDGET (window->entry_variables),
           gettext ("All simulated results file"));
04207
04208
04209
        // Creating the files grid and attaching widgets
        window->grid_files = (GtkGrid *) gtk_grid_new ();
04210
04211
        gtk_grid_attach (window->grid_files, GTK_WIDGET (window->
      label_simulator),
04212
                          0, 0, 1, 1);
        gtk_grid_attach (window->grid_files, GTK_WIDGET (window->
04213
      button_simulator),
                          1, 0, 1, 1);
04215
        gtk_grid_attach (window->grid_files, GTK_WIDGET (window->
      check_evaluator),
04216
                          2, 0, 1, 1);
04217
        gtk_grid_attach (window->grid_files, GTK_WIDGET (window->
```

```
button_evaluator),
                          3, 0, 1, 1);
04218
04219
        gtk_grid_attach (window->grid_files, GTK_WIDGET (window->
      label_result),
04220
                          0, 1, 1, 1);
        gtk_grid_attach (window->grid_files, GTK_WIDGET (window->
04221
      entry_result),
04222
                          1, 1, 1, 1);
        gtk_grid_attach (window->grid_files, GTK_WIDGET (window->
04223
      label_variables),
04224
                          2. 1. 1. 1);
        gtk_grid_attach (window->grid_files, GTK_WIDGET (window->
04225
      entry variables),
04226
                          3, 1, 1, 1);
04227
        \ensuremath{//} Creating the algorithm properties
04228
        window->label_simulations = (GtkLabel *) gtk_label_new
04229
          (gettext ("Simulations number"));
04230
04231
        window->spin_simulations
04232
          = (GtkSpinButton *) gtk_spin_button_new_with_range (1., 1.e12, 1.);
04233
        gtk_widget_set_tooltip_text
          (GTK_WIDGET (window->spin_simulations),
gettext ("Number of simulations to perform for each iteration"));
04234
04235
04236
        window->label iterations = (GtkLabel *)
04237
          qtk_label_new (gettext ("Iterations number"));
        window->spin_iterations
04238
04239
          = (GtkSpinButton *) gtk_spin_button_new_with_range (1., 1.e6, 1.);
        gtk_widget_set_tooltip_text
04240
04241
          (GTK_WIDGET (window->spin_iterations), gettext ("Number of iterations"));
04242
        g_signal_connect
          (window->spin_iterations, "value-changed", window_update, NULL);
04243
04244
        window->label_tolerance = (GtkLabel *) gtk_label_new (gettext ("Tolerance"));
04245
        window->spin_tolerance
04246
          = (GtkSpinButton *) gtk_spin_button_new_with_range (0., 1., 0.001);
04247
        {\tt gtk\_widget\_set\_tooltip\_text}
04248
          (GTK_WIDGET (window->spin_tolerance),
           gettext ("Tolerance to set the variable interval on the next iteration"));
04249
        window->label_bests = (GtkLabel *) gtk_label_new (gettext ("Bests number"));
04250
04251
        window->spin bests
04252
          = (GtkSpinButton *) gtk_spin_button_new_with_range (1., 1.e6, 1.);
04253
        gtk_widget_set_tooltip_text
04254
          (GTK_WIDGET (window->spin_bests),
           gettext ("Number of best simulations used to set the variable interval "
    "on the next iteration"));
04255
04256
        window->label_population
04257
04258
          = (GtkLabel *) gtk_label_new (gettext ("Population number"));
04259
        window->spin_population
04260
          = (GtkSpinButton *) gtk_spin_button_new_with_range (1., 1.e12, 1.);
        gtk_widget_set_tooltip_text
(GTK_WIDGET (window->spin_population),
04261
04262
04263
           gettext ("Number of population for the genetic algorithm"));
04264
        window->label_generations
04265
          = (GtkLabel *) gtk_label_new (gettext ("Generations number"));
04266
        window->spin_generations
          = (GtkSpinButton *) gtk_spin_button_new_with_range (1., 1.e6, 1.);
04267
        gtk_widget_set_tooltip_text
04268
          (GTK_WIDGET (window->spin_generations),
04269
04270
           gettext ("Number of generations for the genetic algorithm"));
04271
        window->label_mutation
04272
          = (GtkLabel *) gtk_label_new (gettext ("Mutation ratio"));
        window->spin mutation
04273
04274
          = (GtkSpinButton *) gtk_spin_button_new_with_range (0., 1., 0.001);
04275
        gtk_widget_set_tooltip_text
04276
          (GTK_WIDGET (window->spin_mutation),
04277
           gettext ("Ratio of mutation for the genetic algorithm"));
04278
        window->label_reproduction
04279
          = (GtkLabel *) gtk_label_new (gettext ("Reproduction ratio"));
04280
        window->spin reproduction
04281
          = (GtkSpinButton *) gtk_spin_button_new_with_range (0., 1., 0.001);
04282
        gtk_widget_set_tooltip_text
04283
          (GTK_WIDGET (window->spin_reproduction),
04284
           gettext ("Ratio of reproduction for the genetic algorithm"));
04285
        window->label_adaptation
          = (GtkLabel *) gtk_label_new (gettext ("Adaptation ratio"));
04286
04287
        window->spin adaptation
04288
          = (GtkSpinButton *) gtk_spin_button_new_with_range (0., 1., 0.001);
04289
        gtk_widget_set_tooltip_text
04290
          (GTK_WIDGET (window->spin_adaptation),
04291
           gettext ("Ratio of adaptation for the genetic algorithm"));
04292
        // Creating the gradient based method properties
04293
04294
        window->check_gradient = (GtkCheckButton *)
04295
          gtk_check_button_new_with_mnemonic (gettext ("_Gradient based method"));
04296
        g_signal_connect (window->check_gradient, "clicked",
      window_update, NULL);
        window->grid_gradient = (GtkGrid *) gtk_grid_new ();
04297
        window->button_gradient[0] = (GtkRadioButton *)
04298
```

```
gtk_radio_button_new_with_mnemonic (NULL, label_gradient[0]);
04300
        gtk_grid_attach (window->grid_gradient,
04301
                         GTK_WIDGET (window->button_gradient[0]), 0, 0, 1, 1);
04302
        g_signal_connect (window->button_gradient[0], "clicked",
      window_update, NULL);
  for (i = 0; ++i < NGRADIENTS;)</pre>
04303
04304
04305
            window->button_gradient[i] = (GtkRadioButton *)
04306
              gtk_radio_button_new_with_mnemonic
04307
               (gtk_radio_button_get_group (window->button_gradient[0]),
04308
               label_gradient[i]);
            gtk_widget_set_tooltip_text (GTK_WIDGET (window->button_gradient[i]),
04309
04310
            tip_gradient[i]);
gtk_grid_attach (window->grid_gradient,
04311
04312
                             GTK_WIDGET (window->button_gradient[i]), 0, i, 1, 1);
04313
            g_signal_connect (window->button_gradient[i], "clicked",
04314
                              window_update, NULL);
04315
04316
        window->label_steps = (GtkLabel *) gtk_label_new (gettext ("Steps number"));
04317
        window->spin_steps = (GtkSpinButton *)
04318
          gtk_spin_button_new_with_range (1., 1.e12, 1.);
04319
        window->label_estimates
04320
          = (GtkLabel *) gtk_label_new (gettext ("Gradient estimates number"));
        window->spin estimates = (GtkSpinButton *)
04321
04322
          gtk_spin_button_new_with_range (1., 1.e3, 1.);
04323
        window->label_relaxation
04324
          = (GtkLabel *) gtk_label_new (gettext ("Relaxation parameter"));
        window->spin_relaxation = (GtkSpinButton *)
04325
04326
         gtk_spin_button_new_with_range (0., 2., 0.001);
04327
        gtk_grid_attach (window->grid_gradient, GTK_WIDGET (window->
      label_steps),
04328
                         0, NGRADIENTS, 1, 1);
        gtk_grid_attach (window->grid_gradient, GTK_WIDGET (window->
04329
      spin_steps),
                         1, NGRADIENTS, 1, 1);
04330
        gtk_grid_attach (window->grid_gradient, GTK_WIDGET (window->
04331
      label_estimates),
04332
                         0, NGRADIENTS + 1, 1, 1);
04333
        gtk_grid_attach (window->grid_gradient, GTK_WIDGET (window->
      spin_estimates),
04334
                         1, NGRADIENTS + 1, 1, 1);
04335
        gtk_grid_attach (window->grid_gradient, GTK_WIDGET (window->
      label_relaxation),
04336
                         0, NGRADIENTS + 2, 1, 1);
04337
        gtk_grid_attach (window->grid_gradient, GTK_WIDGET (window->
      spin_relaxation),
04338
                         1, NGRADIENTS + 2, 1, 1);
04339
        // Creating the array of algorithms
04340
        window->grid_algorithm = (GtkGrid *) gtk_grid_new ();
04341
        window->button_algorithm[0] = (GtkRadioButton *)
04342
04343
          gtk_radio_button_new_with_mnemonic (NULL, label_algorithm[0]);
04344
        gtk_widget_set_tooltip_text (GTK_WIDGET (window->button_algorithm[0]),
04345
                                     tip_algorithm[0]);
04346
        gtk_grid_attach (window->grid_algorithm,
                         GTK_WIDGET (window->button_algorithm[0]), 0, 0, 1, 1);
04347
        g_signal_connect (window->button_algorithm[0], "clicked",
04348
                           window_set_algorithm, NULL);
04349
04350
        for (i = 0; ++i < NALGORITHMS;)</pre>
04351
04352
            window->button algorithm[i] = (GtkRadioButton *)
04353
              gtk radio button new with mnemonic
04354
              (gtk_radio_button_get_group (window->button_algorithm[0]),
               label_algorithm[i]);
04355
            gtk_widget_set_tooltip_text (GTK_WIDGET (window->button_algorithm[i]),
04356
04357
                                          tip_algorithm[i]);
04358
            gtk_grid_attach (window->grid_algorithm,
                             GTK_WIDGET (window->button_algorithm[i]), 0, i, 1, 1);
04359
            g_signal_connect (window->button_algorithm[i], "clicked",
04360
04361
                              window_set_algorithm, NULL);
04362
04363
        gtk_grid_attach (window->grid_algorithm,
04364
                         GTK_WIDGET (window->label_simulations), 0,
04365
        NALGORITHMS, 1, 1); gtk_grid_attach (window->grid_algorithm,
04366
                         GTK_WIDGET (window->spin_simulations), 1, NALGORITHMS, 1, 1);
04367
        gtk_grid_attach (window->grid_algorithm,
04368
04369
                         GTK_WIDGET (window->label_iterations), 0,
04370
                         NALGORITHMS + 1, 1, 1);
04371
        04372
                         NALGORITHMS + 1, 1, 1);
04373
04374
        gtk_grid_attach (window->grid_algorithm,
04375
                         GTK_WIDGET (window->label_tolerance), 0,
04376
                         NALGORITHMS + 2, 1, 1);
04377
        gtk_grid_attach (window->grid_algorithm,
04378
                         GTK_WIDGET (window->spin_tolerance), 1,
```

```
NALGORITHMS + 2, 1, 1);
04379
04380
        gtk_grid_attach (window->grid_algorithm,
04381
                          GTK_WIDGET (window->label_bests), 0, NALGORITHMS + 3, 1, 1);
04382
        gtk_grid_attach (window->grid_algorithm,
                          GTK_WIDGET (window->spin_bests), 1, NALGORITHMS + 3, 1, 1);
04383
04384
        gtk grid attach (window->grid algorithm,
                          GTK_WIDGET (window->label_population), 0,
04385
04386
                          NALGORITHMS + 4, 1, 1);
04387
        gtk_grid_attach (window->grid_algorithm,
                         GTK_WIDGET (window->spin_population), 1,
NALGORITHMS + 4, 1, 1);
04388
04389
        gtk_grid_attach (window->grid_algorithm,
04390
04391
                          GTK_WIDGET (window->label_generations), 0,
                          NALGORITHMS + 5, 1, 1);
04392
04393
        gtk_grid_attach (window->grid_algorithm,
04394
                          GTK_WIDGET (window->spin_generations), 1,
04395
                          NALGORITHMS + 5, 1, 1);
04396
        gtk grid attach (window->grid algorithm,
                          GTK_WIDGET (window->label_mutation), 0,
04397
04398
                          NALGORITHMS + 6, 1, 1);
04399
        gtk_grid_attach (window->grid_algorithm,
04400
                          GTK_WIDGET (window->spin_mutation), 1,
04401
                          NALGORITHMS + 6, 1, 1);
        gtk_grid_attach (window->grid_algorithm,
04402
04403
                          GTK_WIDGET (window->label_reproduction), 0,
                          NALGORITHMS + 7, 1, 1);
04404
        gtk_grid_attach (window->grid_algorithm,
04405
04406
                          GTK_WIDGET (window->spin_reproduction), 1,
04407
                          NALGORITHMS + 7, 1, 1);
        gtk_grid_attach (window->grid_algorithm,
04408
04409
                          GTK_WIDGET (window->label_adaptation), 0,
04410
                          NALGORITHMS + 8, 1, 1);
04411
        gtk_grid_attach (window->grid_algorithm,
04412
                          GTK_WIDGET (window->spin_adaptation), 1,
04413
                          NALGORITHMS + 8, 1, 1);
04414
        gtk_grid_attach (window->grid_algorithm,
                          GTK_WIDGET (window->check_gradient), 0,
04415
                          NALGORITHMS + 9, 2, 1);
04416
04417
        gtk_grid_attach (window->grid_algorithm,
04418
                          GTK_WIDGET (window->grid_gradient), 0,
04419
                         NALGORITHMS + 10, 2, 1);
        \label{limits} \verb|window-> frame\_algorithm = (GtkFrame *) gtk\_frame\_new (gettext ("Algorithm")); \\
04420
        gtk_container_add (GTK_CONTAINER (window->frame_algorithm),
04421
04422
                            GTK_WIDGET (window->grid_algorithm));
04423
04424
        // Creating the variable widgets
04425
        window->combo_variable = (GtkComboBoxText *) gtk_combo_box_text_new ();
04426
        gtk_widget_set_tooltip_text
04427
          (GTK_WIDGET (window->combo_variable), gettext ("Variables selector"));
04428
        window->id_variable = g_signal_connect
04429
          (window->combo_variable, "changed", window_set_variable, NULL);
        window->button_add_variable
04430
04431
          = (GtkButton *) gtk_button_new_from_icon_name ("list-add",
04432
                                                           GTK_ICON_SIZE_BUTTON);
        g_signal_connect
04433
04434
          (window->button add variable, "clicked",
     window_add_variable, NULL);
04435
       atk widget set tooltip text
04436
          (GTK_WIDGET (window->button_add_variable), gettext ("Add variable"));
04437
        window->button_remove_variable
04438
          = (GtkButton *) gtk_button_new_from_icon_name ("list-remove",
04439
                                                           GTK ICON SIZE BUTTON);
04440
       q_signal_connect
04441
          (window->button_remove_variable, "clicked",
      window_remove_variable, NULL);
04442
        gtk_widget_set_tooltip_text
          (GTK_WIDGET (window->button_remove_variable), gettext ("Remove variable"));
04443
        window->label_variable = (GtkLabel *) gtk_label_new (gettext ("Name"));
04444
        window->entry_variable = (GtkEntry *) gtk_entry_new ();
04445
04446
        gtk_widget_set_tooltip_text
04447
          (GTK_WIDGET (window->entry_variable), gettext ("Variable name"));
        window->id_variable_label = g_signal_connect
  (window->entry_variable, "changed", window_label_variable, NULL);
04448
04449
        window->label_min = (GtkLabel *) gtk_label_new (gettext ("Minimum"));
04450
        window->spin_min = (GtkSpinButton *) gtk_spin_button_new_with_range
04451
04452
          (-G_MAXDOUBLE, G_MAXDOUBLE, precision[DEFAULT_PRECISION]);
04453
        gtk_widget_set_tooltip_text
04454
          (GTK_WIDGET (window->spin_min),
04455
           gettext ("Minimum initial value of the variable"));
04456
        viewport = (GtkViewport *) gtk_viewport_new (NULL, NULL);
04457
        gtk_container_add (GTK_CONTAINER (viewport), GTK_WIDGET (window->spin_min));
04458
        window->scrolled_min
04459
          = (GtkScrolledWindow *) gtk_scrolled_window_new (NULL, NULL);
04460
        gtk_container_add (GTK_CONTAINER (window->scrolled_min),
        GTK_WIDGET (viewport));
g_signal_connect (window->spin_min, "value-changed",
04461
04462
04463
                           window_rangemin_variable, NULL);
```

```
04464
        window->label_max = (GtkLabel *) gtk_label_new (gettext ("Maximum"));
        window->spin_max = (GtkSpinButton *) gtk_spin_button_new_with_range
04465
04466
           (-G_MAXDOUBLE, G_MAXDOUBLE, precision[DEFAULT_PRECISION]);
04467
        gtk_widget_set_tooltip_text
04468
          (GTK WIDGET (window->spin max),
04469
           gettext ("Maximum initial value of the variable"));
        viewport = (GtkViewport *) gtk_viewport_new (NULL, NULL);
04470
04471
        gtk_container_add (GTK_CONTAINER (viewport), GTK_WIDGET (window->spin_max));
04472
        window->scrolled_max
04473
          = (GtkScrolledWindow *) gtk_scrolled_window_new (NULL, NULL);
        gtk_container_add (GTK_CONTAINER (window->scrolled_max),
04474
04475
                            GTK_WIDGET (viewport));
04476
        g_signal_connect (window->spin_max, "value-changed",
                            window_rangemax_variable, NULL);
04477
04478
        window->check_minabs = (GtkCheckButton *)
        gtk_check_button_new_with_mnemonic (gettext ("_Absolute minimum"));
g_signal_connect (window->check_minabs, "toggled", window_update, NULL);
window->spin_minabs = (GtkSpinButton *) gtk_spin_button_new_with_range
04479
04480
04481
          (-G_MAXDOUBLE, G_MAXDOUBLE, precision[DEFAULT_PRECISION]);
04482
04483
        gtk_widget_set_tooltip_text
04484
           (GTK_WIDGET (window->spin_minabs),
04485
           gettext ("Minimum allowed value of the variable"));
        \label{eq:viewport} \begin{tabular}{ll} viewport & (GtkViewport *) & gtk_viewport_new & (NULL, NULL); \\ gtk_container_add & (GTK_CONTAINER & (viewport), \\ \end{tabular}
04486
04487
04488
                            GTK_WIDGET (window->spin_minabs));
04489
        window->scrolled_minabs
04490
           = (GtkScrolledWindow *) gtk_scrolled_window_new (NULL, NULL);
04491
        gtk_container_add (GTK_CONTAINER (window->scrolled_minabs),
        04492
04493
04494
04495
        window->check_maxabs = (GtkCheckButton *)
04496
          gtk_check_button_new_with_mnemonic (gettext ("_Absolute maximum"));
04497
        g_signal_connect (window->check_maxabs, "toggled", window_update, NULL);
04498
        \verb|window->spin_maxabs| = (GtkSpinButton *) | gtk_spin_button_new_with_range|
          (-G_MAXDOUBLE, G_MAXDOUBLE, precision[DEFAULT_PRECISION]);
04499
        gtk_widget_set_tooltip_text
04500
04501
          (GTK_WIDGET (window->spin_maxabs),
04502
           gettext ("Maximum allowed value of the variable"));
04503
        viewport = (GtkViewport *) gtk_viewport_new (NULL, NULL);
04504
        gtk_container_add (GTK_CONTAINER (viewport),
04505
                            GTK_WIDGET (window->spin_maxabs));
04506
        window->scrolled maxabs
04507
          = (GtkScrolledWindow *) gtk_scrolled_window_new (NULL, NULL);
        gtk_container_add (GTK_CONTAINER (window->scrolled_maxabs),
04508
04509
                            GTK_WIDGET (viewport));
04510
        g_signal_connect (window->spin_maxabs, "value-changed",
04511
                           window_rangemaxabs_variable, NULL);
04512
        window->label precision
04513
          = (GtkLabel *) gtk label new (gettext ("Precision digits"));
04514
        window->spin_precision = (GtkSpinButton *)
04515
          gtk_spin_button_new_with_range (0., (gdouble) DEFAULT_PRECISION, 1.);
04516
        gtk_widget_set_tooltip_text
04517
           (GTK_WIDGET (window->spin_precision),
04518
           gettext ("Number of precision floating point digits \n"
                     "0 is for integer numbers"));
04519
        g_signal_connect (window->spin_precision, "value-changed",
04520
                           window_precision_variable, NULL);
04521
04522
        window->label_sweeps = (GtkLabel *) gtk_label_new (gettext ("Sweeps number"));
04523
        window->spin_sweeps
          = (GtkSpinButton *) gtk_spin_button_new_with_range (1., 1.e12, 1.);
04524
04525
        gtk_widget_set_tooltip_text
04526
           (GTK_WIDGET (window->spin_sweeps),
           gettext ("Number of steps sweeping the variable"));
04527
04528
        g_signal_connect
04529
           (window->spin_sweeps, "value-changed", window_update_variable, NULL);
04530
        window->label_bits = (GtkLabel *) gtk_label_new (gettext ("Bits number"));
04531
        window->spin bits
04532
          = (GtkSpinButton *) gtk_spin_button_new_with_range (1., 64., 1.);
04533
        gtk_widget_set_tooltip_text
04534
           (GTK_WIDGET (window->spin_bits),
04535
           gettext ("Number of bits to encode the variable"));
04536
        g_signal_connect
          (window->spin_bits, "value-changed", window_update_variable, NULL);
04537
        window->grid_variable = (GtkGrid *) gtk_grid_new ();
gtk_grid_attach (window->grid_variable,
04538
04539
04540
                          GTK_WIDGET (window->combo_variable), 0, 0, 2, 1);
04541
        gtk_grid_attach (window->grid_variable,
04542
                          GTK_WIDGET (window->button_add_variable), 2, 0, 1, 1);
04543
        gtk grid attach (window->grid variable,
                          GTK_WIDGET (window->button_remove_variable), 3, 0, 1, 1);
04544
04545
        gtk_grid_attach (window->grid_variable,
04546
                          GTK_WIDGET (window->label_variable), 0, 1, 1, 1);
04547
        gtk_grid_attach (window->grid_variable,
04548
                          GTK_WIDGET (window->entry_variable), 1, 1, 3, 1);
04549
        gtk_grid_attach (window->grid_variable,
04550
                          GTK_WIDGET (window->label_min), 0, 2, 1, 1);
```

```
gtk_grid_attach (window->grid_variable,
                         GTK_WIDGET (window->scrolled_min), 1, 2, 3, 1);
04552
04553
        gtk_grid_attach (window->grid_variable,
                         GTK_WIDGET (window->label_max), 0, 3, 1, 1);
04554
04555
        gtk_grid_attach (window->grid_variable,
                         GTK_WIDGET (window->scrolled_max), 1, 3, 3, 1);
04556
04557
        gtk_grid_attach (window->grid_variable,
                          GTK_WIDGET (window->check_minabs), 0, 4, 1, 1);
04558
04559
        gtk_grid_attach (window->grid_variable,
04560
                         GTK_WIDGET (window->scrolled_minabs), 1, 4, 3, 1);
        gtk_grid_attach (window->grid_variable,
04561
                         GTK WIDGET (window->check maxabs), 0, 5, 1, 1);
04562
        gtk_grid_attach (window->grid_variable,
04563
04564
                         GTK_WIDGET (window->scrolled_maxabs), 1, 5, 3, 1);
04565
        gtk_grid_attach (window->grid_variable,
04566
                         GTK_WIDGET (window->label_precision), 0, 6, 1, 1);
04567
        gtk_grid_attach (window->grid_variable,
                         GTK WIDGET (window->spin precision), 1, 6, 3, 1);
04568
04569
        gtk_grid_attach (window->grid_variable,
04570
                         GTK_WIDGET (window->label_sweeps), 0, 7, 1, 1);
04571
        gtk_grid_attach (window->grid_variable,
04572
                         GTK_WIDGET (window->spin_sweeps), 1, 7, 3, 1);
        gtk_grid_attach (window->grid_variable,
04573
04574
                         GTK_WIDGET (window->label_bits), 0, 8, 1, 1);
04575
       gtk_grid_attach (window->grid_variable,
                         GTK_WIDGET (window->spin_bits), 1, 8, 3, 1);
04576
04577
        window->frame_variable = (GtkFrame *) gtk_frame_new (gettext ("Variable"));
04578
        gtk_container_add (GTK_CONTAINER (window->frame_variable),
04579
                           GTK_WIDGET (window->grid_variable));
04580
04581
        // Creating the experiment widgets
04582
        window->combo_experiment = (GtkComboBoxText *) gtk_combo_box_text_new ();
04583
        gtk_widget_set_tooltip_text (GTK_WIDGET (window->combo_experiment),
04584
                                      gettext ("Experiment selector"));
        window->id_experiment = g_signal_connect
  (window->combo_experiment, "changed", window_set_experiment, NULL)
04585
04586
04587
       window->button_add_experiment
04588
          = (GtkButton *) gtk_button_new_from_icon_name ("list-add",
04589
                                                          GTK_ICON_SIZE_BUTTON);
04590
        g_signal_connect
04591
          (window->button_add_experiment, "clicked",
     window add experiment, NULL):
04592
        gtk_widget_set_tooltip_text (GTK_WIDGET (window->button_add_experiment),
04593
                                     gettext ("Add experiment"));
04594
        window->button_remove_experiment
04595
          = (GtkButton *) gtk_button_new_from_icon_name ("list-remove",
04596
                                                         GTK_ICON_SIZE_BUTTON);
04597
        q_signal_connect (window->button_remove_experiment, "clicked",
04598
                          window remove experiment, NULL);
04599
        gtk_widget_set_tooltip_text (GTK_WIDGET (window->button_remove_experiment),
04600
                                     gettext ("Remove experiment"));
04601
        window->label_experiment
04602
          = (GtkLabel *) gtk_label_new (gettext ("Experimental data file"));
        window->button_experiment = (GtkFileChooserButton *)
04603
          gtk_file_chooser_button_new (gettext ("Experimental data file"),
04604
                                        GTK_FILE_CHOOSER_ACTION_OPEN);
04605
        gtk_widget_set_tooltip_text (GTK_WIDGET (window->button_experiment),
04606
04607
                                     gettext ("Experimental data file"));
04608
        window->id_experiment_name
          = g_signal_connect (window->button_experiment, "selection-changed",
04609
04610
                              window name experiment, NULL);
04611
        window->label_weight = (GtkLabel *) gtk_label_new (gettext ("Weight"));
        window->spin_weight
04612
04613
          = (GtkSpinButton *) gtk_spin_button_new_with_range (0., 1., 0.001);
04614
        gtk_widget_set_tooltip_text
04615
          (GTK_WIDGET (window->spin_weight),
           gettext ("Weight factor to build the objective function"));
04616
04617
        g_signal_connect
04618
          (window->spin_weight, "value-changed", window_weight_experiment,
     NULL);
04619
        window->grid_experiment = (GtkGrid *) gtk_grid_new ();
04620
        gtk_grid_attach (window->grid_experiment,
04621
                         GTK WIDGET (window->combo_experiment), 0, 0, 2, 1);
        gtk grid attach (window->grid experiment,
04622
                         GTK_WIDGET (window->button_add_experiment), 2, 0, 1, 1);
04623
04624
        gtk_grid_attach (window->grid_experiment,
04625
                         GTK_WIDGET (window->button_remove_experiment), 3, 0, 1, 1);
04626
        gtk_grid_attach (window->grid_experiment,
                         GTK WIDGET (window->label_experiment), 0, 1, 1, 1);
04627
04628
        gtk_grid_attach (window->grid_experiment,
04629
                         GTK_WIDGET (window->button_experiment), 1, 1, 3, 1);
        gtk_grid_attach (window->grid_experiment,
04630
04631
                         GTK_WIDGET (window->label_weight), 0, 2, 1, 1);
04632
        gtk_grid_attach (window->grid_experiment,
04633
                         GTK_WIDGET (window->spin_weight), 1, 2, 3, 1);
        for (i = 0; i < MAX_NINPUTS; ++i)</pre>
04634
```

```
snprintf (buffer3, 64, "%s %u", gettext ("Input template"), i + 1);
04636
04637
            window->check_template[i] = (GtkCheckButton *)
              gtk_check_button_new_with_label (buffer3);
04638
04639
            window->id template[i]
              = q_signal_connect (window->check_template[i], "toggled",
04640
04641
                                   window_inputs_experiment, NULL);
04642
            gtk_grid_attach (window->grid_experiment,
            GTK_WIDGET (window->check_template[i]), 0, 3 + i, 1, 1);
window->button_template[i] = (GtkFileChooserButton *)
04643
04644
              04645
04646
04647
            gtk_widget_set_tooltip_text
04648
              (GTK_WIDGET (window->button_template[i]),
04649
               gettext ("Experimental input template file"));
04650
            window->id_input[i]
04651
              = q_signal_connect_swapped (window->button_template[i],
                                            "selection-changed",
(void (*)) window_template_experiment,
04652
04653
04654
                                            (void *) (size_t) i);
04655
            gtk_grid_attach (window->grid_experiment,
04656
                              GTK_WIDGET (window->button_template[i]), 1, 3 + i, 3, 1);
04657
        window->frame_experiment
04658
04659
          = (GtkFrame *) gtk_frame_new (gettext ("Experiment"));
        gtk_container_add (GTK_CONTAINER (window->frame_experiment),
04660
04661
                            GTK_WIDGET (window->grid_experiment));
04662
04663
        // Creating the grid and attaching the widgets to the grid
04664
        window->grid = (GtkGrid \star) gtk_grid_new ();
        gtk_grid_attach (window->grid, GTK_WIDGET (window->bar_buttons), 0, 0, 3, 1);
gtk_grid_attach (window->grid, GTK_WIDGET (window->grid_files), 0, 1, 3, 1);
04665
04666
04667
        gtk_grid_attach (window->grid,
04668
                          GTK_WIDGET (window->frame_algorithm), 0, 2, 1, 1);
04669
        gtk_grid_attach (window->grid,
                          GTK WIDGET (window->frame variable), 1, 2, 1, 1);
04670
04671
        gtk grid attach (window->grid,
                          GTK_WIDGET (window->frame_experiment), 2, 2, 1, 1);
04672
04673
        gtk_container_add (GTK_CONTAINER (window->window), GTK_WIDGET (window->
04674
04675
        // Setting the window logo
04676
        window->logo = gdk_pixbuf_new_from_xpm_data (logo);
04677
        gtk_window_set_icon (window->window, window->logo);
04678
04679
        // Showing the window
04680
        gtk_widget_show_all (GTK_WIDGET (window->window));
04681
04682
        // In GTK+ 3.16 and 3.18 the default scrolled size is wrong
04683 #if GTK_MINOR_VERSION >= 16
04684
        gtk_widget_set_size_request (GTK_WIDGET (window->scrolled_min), -1, 40);
04685
        gtk_widget_set_size_request (GTK_WIDGET (window->scrolled_max), -1, 40);
04686
        gtk_widget_set_size_request (GTK_WIDGET (window->scrolled_minabs), -1, 40);
04687
        gtk_widget_set_size_request (GTK_WIDGET (window->scrolled_maxabs), -1, 40);
04688 #endif
04689
04690
        // Reading initial example
04691
        input_new ();
04692
        buffer2 = g_get_current_dir ();
        buffer = g_build_filename (buffer2, "...", "tests", "test1", INPUT_FILE, NULL);
04693
        g_free (buffer2);
04694
04695
       window_read (buffer);
04696
       g_free (buffer);
04697 }
04698
04699 #endif
04700
04706 int
04707 cores_number ()
04708 {
04709 #ifdef G_OS_WIN32
04710 SYSTEM_INFO sysinfo;
04711 GetSystemInfo (&sysinfo);
04712
        return sysinfo.dwNumberOfProcessors;
04713 #else
04714 return (int) sysconf (_SC_NPROCESSORS_ONLN);
04715 #endif
04716 }
04717
04727 int.
04728 main (int argn, char **argc)
04730 #if HAVE_GTK
04731
       char *buffer;
04732 #endif
04733
04734
       // Starting pseudo-random numbers generator
```

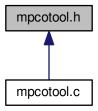
```
calibrate->rng = gsl_rng_alloc (gsl_rng_taus2);
04736
        calibrate->seed = DEFAULT_RANDOM_SEED;
04737
04738
        \ensuremath{//} Allowing spaces in the XML data file
04739
        xmlKeepBlanksDefault (0);
04740
04741
         // Starting MPI
04742 #if HAVE_MPI
04743 MPI_Init (&argn, &argc);
       MPI_Comm_size (MPI_COMM_WORLD, &ntasks);
MPI_Comm_rank (MPI_COMM_WORLD, &calibrate->mpi_rank);
printf ("rank=%d tasks=%d\n", calibrate->mpi_rank, ntasks);
04744
04745
04746
04747 #else
04748 \quad \text{ntasks} = 1;
04749 #endif
04750
04751 #if HAVE GTK
04752
04753
        // Getting threads number
04754
        nthreads_gradient = nthreads = cores_number ();
04755
04756
        \ensuremath{//} Setting local language and international floating point numbers notation
        setlocale (LC_ALL, "");
setlocale (LC_NUMERIC, "C");
04757
04758
04759
        window->application_directory = g_get_current_dir ();
        buffer = g_build_filename (window->application_directory,
04760
      LOCALE_DIR, NULL);
04761
        bindtextdomain (PROGRAM_INTERFACE, buffer);
        bind_textdomain_codeset (PROGRAM_INTERFACE, "UTF-8");
textdomain (PROGRAM_INTERFACE);
04762
04763
04764
04765
        // Initing GTK+
04766
        gtk_disable_setlocale ();
04767
        gtk_init (&argn, &argc);
04768
        // Opening the main window
04769
04770
        window_new ();
04771
        gtk_main ();
04772
04773
        // Freeing memory
04774
        input_free ();
04775
        g_free (buffer);
04776
        gtk_widget_destroy (GTK_WIDGET (window->window));
04777
        g_free (window->application_directory);
04778
04779 #else
04780
04781
        // Checking syntax
        if (!(argn == 2 || (argn == 4 && !strcmp (argc[1], "-nthreads"))))
04782
04783
04784
             printf ("The syntax is:\nmpcotoolbin [-nthreads x] data_file\n");
04785
04786
          }
04787
04788
        // Getting threads number
04789
        if (argn == 2)
04790
          nthreads_gradient = nthreads = cores_number ();
04791
        else
04792
04793
             nthreads_gradient = nthreads = atoi (argc[2]);
04794
             if (!nthreads)
04795
04796
                 printf ("Bad threads number\n");
04797
                 return 2;
04798
04799
04800
        printf ("nthreads=%u\n", nthreads);
04801
04802
        // Making calibration
04803
        if (input_open (argc[argn - 1]))
04804
          calibrate_open ();
04805
04806
        // Freeing memory
04807
        calibrate_free ();
04808
04809 #endif
04810
04811
        // Closing MPI
04812 #if HAVE_MPI
        MPI Finalize ();
04813
04814 #endif
04815
04816
         // Freeing memory
04817
        gsl_rng_free (calibrate->rng);
04818
        // Closing
04819
04820
        return 0;
```

04821 }

5.7 mpcotool.h File Reference

Header file of the mpcotool.

This graph shows which files directly or indirectly include this file:



Data Structures

struct Input

Struct to define the calibration input file.

struct Calibrate

Struct to define the calibration data.

struct ParallelData

Struct to pass to the GThreads parallelized function.

Enumerations

```
    enum Algorithm { ALGORITHM_MONTE_CARLO = 0, ALGORITHM_SWEEP = 1, ALGORITHM_GENETIC = 2 }
```

Enum to define the algorithms.

enum GradientMethod { GRADIENT_METHOD_COORDINATES = 0, GRADIENT_METHOD_RANDOM = 1 }

Enum to define the methods to estimate the gradient.

Functions

• void show_message (char *title, char *msg, int type)

Function to show a dialog with a message.

void show error (char *msg)

Function to show a dialog with an error message.

int xml_node_get_int (xmlNode *node, const xmlChar *prop, int *error_code)

Function to get an integer number of a XML node property.

unsigned int xml_node_get_uint (xmlNode *node, const xmlChar *prop, int *error_code)

Function to get an unsigned integer number of a XML node property.

double xml_node_get_float (xmlNode *node, const xmlChar *prop, int *error_code)

Function to get a floating point number of a XML node property.

void xml_node_set_int (xmlNode *node, const xmlChar *prop, int value)

Function to set an integer number in a XML node property.

void xml node set uint (xmlNode *node, const xmlChar *prop, unsigned int value)

Function to set an unsigned integer number in a XML node property.

• void xml_node_set_float (xmlNode *node, const xmlChar *prop, double value)

Function to set a floating point number in a XML node property.

· void input new ()

Function to create a new Input struct.

· void input_free ()

Function to free the memory of the input file data.

int input open (char *filename)

Function to open the input file.

void calibrate_input (unsigned int simulation, char *input, GMappedFile *template)

Function to write the simulation input file.

double calibrate_parse (unsigned int simulation, unsigned int experiment)

Function to parse input files, simulating and calculating the \ objective function.

• void calibrate print ()

Function to print the results.

void calibrate_save_variables (unsigned int simulation, double error)

Function to save in a file the variables and the error.

void calibrate best (unsigned int simulation, double value)

Function to save the best simulations.

void calibrate_sequential ()

Function to calibrate sequentially.

void * calibrate_thread (ParallelData *data)

Function to calibrate on a thread.

void calibrate_merge (unsigned int nsaveds, unsigned int *simulation_best, double *error_best)

Function to merge the 2 calibration results.

• void calibrate_synchronise ()

Function to synchronise the calibration results of MPI tasks.

void calibrate_sweep ()

Function to calibrate with the sweep algorithm.

• void calibrate MonteCarlo ()

Function to calibrate with the Monte-Carlo algorithm.

• void calibrate best gradient (unsigned int simulation, double value)

Function to save the best simulation in a gradient based method.

- void calibrate gradient sequential ()
- void * calibrate_gradient_thread (ParallelData *data)

Function to estimate the gradient on a thread.

- double calibrate variable step gradient (unsigned int variable)
- void calibrate step gradient (unsigned int simulation)

Function to do a step of the gradient based method.

void calibrate_gradient ()

Function to calibrate with a gradient based method.

double calibrate genetic objective (Entity *entity)

Function to calculate the objective function of an entity.

void calibrate_genetic ()

Function to calibrate with the genetic algorithm.

void calibrate_save_old ()

Function to save the best results on iterative methods.

void calibrate_merge_old ()

Function to merge the best results with the previous step best results on iterative methods.

• void calibrate_refine ()

Function to refine the search ranges of the variables in iterative algorithms.

void calibrate_step ()

Function to do a step of the iterative algorithm.

void calibrate_iterate ()

Function to iterate the algorithm.

• void calibrate open ()

Function to open and perform a calibration.

5.7.1 Detailed Description

Header file of the mpcotool.

Authors

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Definition in file mpcotool.h.

5.7.2 Enumeration Type Documentation

5.7.2.1 enum Algorithm

Enum to define the algorithms.

Enumerator

ALGORITHM_MONTE_CARLO Monte-Carlo algorithm. **ALGORITHM_SWEEP** Sweep algorithm. **ALGORITHM_GENETIC** Genetic algorithm.

Definition at line 43 of file mpcotool.h.

5.7.2.2 enum GradientMethod

Enum to define the methods to estimate the gradient.

Enumerator

GRADIENT_METHOD_COORDINATES Coordinates descent method. **GRADIENT_METHOD_RANDOM** Random method.

Definition at line 54 of file mpcotool.h.

```
00055 {
00056    GRADIENT_METHOD_COORDINATES = 0,
00057    GRADIENT_METHOD_RANDOM = 1,
00058 };
```

5.7.3 Function Documentation

5.7.3.1 void calibrate_best (unsigned int *simulation*, double *value*)

Function to save the best simulations.

Parameters

simulation	Simulation number.
value	Objective function value.

Definition at line 1420 of file mpcotool.c.

```
01421 {
01422
        unsigned int i, j;
01423
        double e;
01424 #if DEBUG
01425 fprintf (stderr, "calibrate_best: start\n");
01426 fprintf (stderr, "calibrate_best: nsaveds=%u nbest=%u\n",
01427
                  calibrate->nsaveds, calibrate->nbest);
01428 #endif
01429 if (calibrate->nsaveds < calibrate->nbest
01430
            || value < calibrate->error_best[calibrate->nsaveds - 1])
         {
01431
01432
            if (calibrate->nsaveds < calibrate->nbest)
01433
               ++calibrate->nsaveds;
01434
            calibrate->error_best[calibrate->nsaveds - 1] = value;
01435
            calibrate->simulation_best[calibrate->
     nsaveds - 1] = simulation;
for (i = calibrate->nsaveds; --i;)
01436
01437
              {
                 if (calibrate->error_best[i] < calibrate->
01438
      error_best[i - 1])
01439
01440
                     j = calibrate->simulation_best[i];
01441
                     e = calibrate->error_best[i];
                     calibrate->simulation_best[i] = calibrate->
01442
      simulation_best[i - 1];
                    calibrate->error_best[i] = calibrate->
error_best[i - 1];
01444 cali
                     calibrate->simulation_best[i - 1] = j;
01445
                     calibrate->error_best[i - 1] = e;
                   }
01446
               else
01447
01448
                  break;
01449
01450
01451 #if DEBUG
01452 fprintf (stderr, "calibrate_best: end\n");
01453 #endif
01454 }
```

5.7.3.2 void calibrate_best_gradient (unsigned int simulation, double value)

Function to save the best simulation in a gradient based method.

Parameters

simulation	Simulation number.
value	Objective function value.

Definition at line 1733 of file mpcotool.c.

```
01734 {
01735 #if DEBUG
01736
       fprintf (stderr, "calibrate_best_gradient: start\n");
01737
       fprintf (stderr,
                 "calibrate_best_gradient: simulation=%u value=%.14le best=%.14le\n",
01738
                simulation, value, calibrate->error_best[0]);
01740 #endif
01741 if (value < calibrate->error_best[0])
01742
           calibrate->error_best[0] = value;
01743
01744
           calibrate->simulation_best[0] = simulation;
01745 #if DEBUG
01746
           fprintf (stderr,
```

5.7.3.3 double calibrate_genetic_objective (Entity * entity)

Function to calculate the objective function of an entity.

Parameters

```
entity entity data.
```

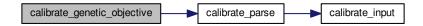
Returns

objective function value.

Definition at line 2036 of file mpcotool.c.

```
02037 {
02038
       unsigned int j;
02039
       double objective;
02040
        char buffer[64];
02042
       fprintf (stderr, "calibrate_genetic_objective: start\n");
02043 #endif
02044
       for (j = 0; j < calibrate->nvariables; ++j)
02045
02046
            calibrate->value[entity->id * calibrate->nvariables + j]
02047
              = genetic_get_variable (entity, calibrate->genetic_variable + j);
02048
02049
       for (j = 0, objective = 0.; j < calibrate->nexperiments; ++j)
02050
         objective += calibrate_parse (entity->id, j);
        g_mutex_lock (mutex);
02051
        for (j = 0; j < calibrate->nvariables; ++j)
02052
02053
02054
            snprintf (buffer, 64, "%s ", format[calibrate->precision[j]]);
02055
            fprintf (calibrate->file_variables, buffer,
02056
                     genetic_get_variable (entity, calibrate->
      genetic_variable + j));
02057
02058
        fprintf (calibrate->file_variables, "%.14le\n", objective);
02059
        g_mutex_unlock (mutex);
02060 #if DEBUG
02061
       fprintf (stderr, "calibrate_genetic_objective: end\n");
02062 #endif
02063
       return objective;
02064 }
```

Here is the call graph for this function:



5.7.3.4 void* calibrate_gradient_thread (ParallelData * data)

Function to estimate the gradient on a thread.

Parameters

data Function data.

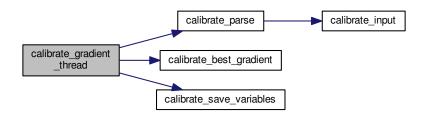
Returns

NULL

Definition at line 1798 of file mpcotool.c.

```
01799 {
01800
        unsigned int i, j, thread;
01801
        double e;
01802 #if DEBUG
        fprintf (stderr, "calibrate_gradient_thread: start\n");
01803
01804 #endif
01805
        thread = data->thread;
01806 #if DEBUG
01807 fprintf (stderr, "calibrate_gradient_thread: thread=%u start=%u end=%un",
01808
                  thread,
                  calibrate->thread_gradient[thread],
calibrate->thread_gradient[thread + 1]);
01809
01810
01811 #endif
        for (i = calibrate->thread_gradient[thread];
01812
01813
              i < calibrate->thread_gradient[thread + 1]; ++i)
01814
            e = 0.;
01815
            for (j = 0; j < calibrate->nexperiments; ++j)
e += calibrate_parse (i, j);
01816
01817
01818
            g_mutex_lock (mutex);
01819
            calibrate_best_gradient (i, e);
01820
            calibrate_save_variables (i, e);
01821
             g_mutex_unlock (mutex);
01822 #if DEBUG
01823
             fprintf (stderr, "calibrate_gradient_thread: i=%u e=%lg\n", i, e);
01824 #endif
01825
01826 #if DEBUG
       fprintf (stderr, "calibrate_gradient_thread: end\n");
01827
01828 #endif
       g_thread_exit (NULL);
01829
01830
        return NULL;
01831 }
```

Here is the call graph for this function:



5.7.3.5 void calibrate input (unsigned int simulation, char * input, GMappedFile * template)

Function to write the simulation input file.

Parameters

simulation	Simulation number.
input	Input file name.
template	Template of the input file name.

Definition at line 1173 of file mpcotool.c.

```
01174 {
       unsigned int i:
01175
01176
       char buffer[32], value[32], *buffer2, *buffer3, *content;
01177
       FILE *file;
01178
       gsize length;
01179
       GRegex *regex;
01180
01181 #if DEBUG
01182
       fprintf (stderr, "calibrate input: start\n");
01183 #endif
01184
       // Checking the file
01185
01186
       if (!template)
01187
        goto calibrate_input_end;
01188
       // Opening template
01189
01190
      content = g_mapped_file_get_contents (template);
01191
       length = g_mapped_file_get_length (template);
01192 #if DEBUG
01193 fprintf (stderr, "calibrate_input: length=%lu\ncontent:\n%s", length,
01194
                content):
01195 #endif
01196
       file = g_fopen (input, "w");
01197
01198
       // Parsing template
01199
      for (i = 0; i < calibrate->nvariables; ++i)
01200
01201 #if DEBUG
01202
           fprintf (stderr, "calibrate_input: variable=%u\n", i);
01203 #endif
01204
          snprintf (buffer, 32, "@variable%u@", i + 1);
01205
           regex = g_regex_new (buffer, 0, 0, NULL);
           if (i == 0)
01206
01207
01208
               buffer2 = g_regex_replace_literal (regex, content, length, 0,
01209
                                                  calibrate->label[i], 0, NULL);
01210 #if DEBUG
01211
              fprintf (stderr, "calibrate_input: buffer2\n%s", buffer2);
01212 #endif
01213
             }
01214
           else
01215
           {
01216
               length = strlen (buffer3);
01217
               buffer2 = g_regex_replace_literal (regex, buffer3, length, 0,
01218
             g_free (buffer3);
}
                                                  calibrate->label[i], 0, NULL);
01219
01220
01221
           g_regex_unref (regex);
01222
           length = strlen (buffer2);
01223
           snprintf (buffer, 32, "@value%u@", i + 1);
           01224
01225
01226
     nvariables + i]);
01227
01228 #if DEBUG
01229 fprintf (stderr, "calibrate_input: value=%s\n", value);
01230 #endif
           buffer3 = g_regex_replace_literal (regex, buffer2, length, 0, value,
01231
01232
                                              0, NULL);
01233
           g_free (buffer2);
01234
           g_regex_unref (regex);
        }
01235
01236
01237
       // Saving input file
01238
       fwrite (buffer3, strlen (buffer3), sizeof (char), file);
01239
       g_free (buffer3);
01240
       fclose (file);
01241
01242 calibrate_input_end:
01243 #if DEBUG
01244
       fprintf (stderr, "calibrate_input: end\n");
01245 #endif
01246
      return;
01247 }
```

5.7.3.6 void calibrate_merge (unsigned int nsaveds, unsigned int * simulation_best, double * error_best)

Function to merge the 2 calibration results.

Parameters

nsaveds	Number of saved results.
simulation_best	Array of best simulation numbers.
error_best	Array of best objective function values.

Definition at line 1538 of file mpcotool.c.

```
01540 {
        unsigned int i, j, k, s[calibrate->nbest];
01541
        double e[calibrate->nbest];
01542
01543 #if DEBUG
        fprintf (stderr, "calibrate_merge: start\n");
01545 #endif
01546   i = j = k = 0;
01547
        do
01548
          {
01549
            if (i == calibrate->nsaveds)
01550
              {
01551
                s[k] = simulation_best[j];
01552
                e[k] = error_best[j];
01553
                ++j;
                ++k;
01554
01555
                if (j == nsaveds)
01556
                  break;
01557
01558
            else if (j == nsaveds)
01559
01560
                s[k] = calibrate->simulation best[i];
                e[k] = calibrate->error_best[i];
01561
01562
                ++i;
01563
                ++k;
01564
                if (i == calibrate->nsaveds)
01565
                  break;
01566
            else if (calibrate->error_best[i] > error_best[j])
01567
01568
                s[k] = simulation_best[j];
01569
01570
                e[k] = error_best[j];
01571
                ++j;
01572
                ++k;
01573
01574
            else
01575
                s[k] = calibrate->simulation_best[i];
e[k] = calibrate->error_best[i];
01576
01577
01578
                ++i;
01579
                ++k:
01580
01581
01582
       while (k < calibrate->nbest);
01583
       calibrate->nsaveds = k;
01584 memcpy (calibrate->simulation_best, s, k \star sizeof (unsigned int));
        memcpy (calibrate->error_best, e, k * sizeof (double));
01585
01586 #if DEBUG
01587 fprintf (stderr, "calibrate_merge: end\n");
01588 #endif
01589 }
```

5.7.3.7 double calibrate_parse (unsigned int simulation, unsigned int experiment)

Function to parse input files, simulating and calculating the $\$ objective function.

Parameters

simulation	Simulation number.
experiment	Experiment number.

Returns

Objective function value.

Definition at line 1260 of file mpcotool.c.

```
01261 {
01262
        unsigned int i:
01263
        double e;
        char buffer[512], input[MAX_NINPUTS][32], output[32], result[32], *buffer2,
01264
01265
          *buffer3, *buffer4;
01266 FILE *file_result;
01267
01268 #if DEBUG
01269 fprintf (stderr, "calibrate_parse: start\n");
01270 fprintf (stderr, "calibrate_parse: simulation=%u experiment=%u\n", simulation,
01271
                  experiment);
01272 #endif
01273
        // Opening input files
for (i = 0; i < calibrate->ninputs; ++i)
01274
01275
01276
             snprintf (&input[i][0], 32, "input-%u-%u-%u", i, simulation, experiment);
01277
01278 #if DEBUG
01279
            fprintf (stderr, "calibrate_parse: i=%u input=%s\n", i, &input[i][0]);
01280 #endif
01281
            calibrate_input (simulation, &input[i][0],
01282
                               calibrate->file[i][experiment]);
01283
01284
        for (; i < MAX_NINPUTS; ++i)</pre>
01285 strepy (&input[i][0], "");
01286 #if DEBUG
01287
        fprintf (stderr, "calibrate_parse: parsing end\n");
01288 #endif
01290
        // Performing the simulation
01291
        snprintf (output, 32, "output-%u-%u", simulation, experiment);
        buffer2 = g_path_get_dirname (calibrate->simulator);
01292
01293
        buffer3 = g_path_get_basename (calibrate->simulator);
01294
        buffer4 = g_build_filename (buffer2, buffer3, NULL);
01295
        snprintf (buffer, 512, "\"%s\" %s %s",
01296
                   buffer4, input[0], input[1], input[2], input[3], input[4], input[5],
01297
                   input[6], input[7], output);
01298
        g_free (buffer4);
01299
        g_free (buffer3);
        g_free (buffer2);
01300
01301 #if DEBUG
01302
        fprintf (stderr, "calibrate_parse: %s\n", buffer);
01303 #endif
01304
        system (buffer);
01305
01306
        // Checking the objective value function
01307
        if (calibrate->evaluator)
01308
          {
01309
             snprintf (result, 32, "result-%u-%u", simulation, experiment);
01310
            buffer2 = g_path_get_dirname (calibrate->evaluator);
            buffer3 = g_path_get_basename (calibrate->evaluator);
01311
            buffer4 = g_build_filename (buffer2, buffer3, NULL); snprintf (buffer, 512, "\"%s\" %s %s %s",
01312
01313
01314
                       buffer4, output, calibrate->experiment[experiment], result);
            g_free (buffer4);
01315
01316
             g_free (buffer3);
01317
             g_free (buffer2);
01318 #if DEBUG
01319
            fprintf (stderr, "calibrate_parse: %s\n", buffer);
01320 #endif
01321
        system (buffer);
01322
            file_result = g_fopen (result, "r");
            e = atof (fgets (buffer, 512, file_result));
fclose (file_result);
01323
01324
01325
01326
        else
01327
         {
01328
            strcpy (result, "");
            file_result = g_fopen (output, "r");
e = atof (fgets (buffer, 512, file_result));
01329
01330
01331
            fclose (file_result);
01332
01333
01334
        // Removing files
01335 #if !DEBUG
       for (i = 0; i < calibrate->ninputs; ++i)
01336
01337
01338
             if (calibrate->file[i][0])
01339
```

```
snprintf (buffer, 512, RM " %s", &input[i][0]);
01341
               system (buffer);
01342
01343
         }
       snprintf (buffer, 512, RM " %s %s", output, result);
01344
       system (buffer);
01345
01346 #endif
01347
01348 #if DEBUG
01349 fprintf (stderr, "calibrate_parse: end\n");
01350 #endif
01351
01352
       // Returning the objective function
01353
       return e * calibrate->weight[experiment];
01354 }
```

Here is the call graph for this function:



5.7.3.8 void calibrate_save_variables (unsigned int simulation, double error)

Function to save in a file the variables and the error.

Parameters

simulatio	Simulation number.
err	or Error value.

Definition at line 1392 of file mpcotool.c.

```
01393 {
       unsigned int i;
01394
       char buffer[64];
01397
       fprintf (stderr, "calibrate_save_variables: start\n");
01398 #endif
01399
      for (i = 0; i < calibrate->nvariables; ++i)
01400
01401
           snprintf (buffer, 64, "%s ", format[calibrate->precision[i]]);
           fprintf (calibrate->file_variables, buffer,
01402
01403
                     calibrate->value[simulation * calibrate->
nvariables + i]);
01404 }
01405
       fprintf (calibrate->file_variables, "%.14le\n", error);
01406 #if DEBUG
       fprintf (stderr, "calibrate_save_variables: end\n");
01408 #endif
01409 }
```

5.7.3.9 void calibrate_step_gradient (unsigned int simulation)

Function to do a step of the gradient based method.

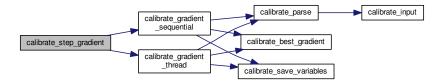
Parameters

simulation | Simulation number.

Definition at line 1900 of file mpcotool.c.

```
01901 {
       GThread *thread[nthreads_gradient];
01902
        ParallelData data[nthreads_gradient];
01903
01904
        unsigned int i, j, k, b;
01905 #if DEBUG
01906
       fprintf (stderr, "calibrate_step_gradient: start\n");
01907 #endif
01908
       for (i = 0; i < calibrate->nestimates: ++i)
01909
01910
            k = (simulation + i) * calibrate->nvariables;
01911
            b = calibrate->simulation_best[0] * calibrate->
      nvariables;
01912 #if DEBUG
           fprintf (stderr, "calibrate_step_gradient: simulation=%u best=%u\n",
01913
01914
                     simulation + i, calibrate->simulation_best[0]);
01915 #endif
           for (j = 0; j < calibrate->nvariables; ++j, ++k, ++b)
01917
01918 #if DEBUG
               fprintf (stderr, "calibrate_step_gradient: estimate=%u best%u=%.14le\n",
01919
01920
01921
                         i, j, calibrate->value[b]);
01922 #endif
               calibrate->value[k]
01923
01924
                  = calibrate->value[b] + calibrate_estimate_gradient (j
, i);
01925
                calibrate->value[k] = fmin (fmax (calibrate->
     value[k].
01926
                                                   calibrate->rangeminabs[j]),
01927
                                             calibrate->rangemaxabs[j]);
01928 #if DEBUG
01929
                fprintf (stderr,
                          "calibrate_step_gradient: estimate=%u variable%u=%.14le\n",
01930
01931
                         i, j, calibrate->value[k]);
01932 #endif
01933
01934
01935
        if (nthreads_gradient == 1)
         calibrate_gradient_sequential (simulation);
01936
01937
        else
01938
         {
01939
            for (i = 0; i <= nthreads_gradient; ++i)</pre>
01940
01941
                calibrate->thread_gradient[i]
01942
                 = simulation + calibrate->nstart_gradient
                  + i * (calibrate->nend_gradient - calibrate->
01943
     nstart_gradient)
01944
                 / nthreads_gradient;
01945 #if DEBUG
01946
                fprintf (stderr,
01947
                          "calibrate_step_gradient: i=%u thread_gradient=%u\n",
01948
                         i, calibrate->thread_gradient[i]);
01949 #endif
01950
01951
            for (i = 0; i < nthreads_gradient; ++i)</pre>
01952
                data[i].thread = i;
01953
               thread[i] = g_thread_new
01954
01955
                 (NULL, (void (*)) calibrate_gradient_thread, &data[i]);
01956
01957
            for (i = 0; i < nthreads_gradient; ++i)</pre>
01958
             g_thread_join (thread[i]);
01959
01960 #if DEBUG
01961
       fprintf (stderr, "calibrate_step_gradient: end\n");
01962 #endif
01963 }
```

Here is the call graph for this function:



5.7.3.10 void* calibrate_thread (ParallelData * data)

Function to calibrate on a thread.

Parameters

```
data Function data.
```

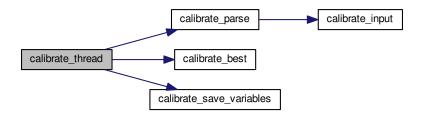
Returns

NULL

Definition at line 1494 of file mpcotool.c.

```
01495 {
        unsigned int i, j, thread;
01496
01497
        double e;
01498 #if DEBUG
01499
       fprintf (stderr, "calibrate_thread: start\n");
01500 #endif
01501
        thread = data->thread;
01502 #if DEBUG
        fprintf (stderr, "calibrate_thread: thread=%u start=%u end=%u\n", thread,
01503
01504
                 calibrate->thread[thread], calibrate->thread[thread + 1]);
01505 #endif
01506
       for (i = calibrate->thread[thread]; i < calibrate->thread[thread + 1]; ++i)
01507
01508
            e = 0.;
            for (j = 0; j < calibrate->nexperiments; ++j)
  e += calibrate_parse (i, j);
01509
01510
            g_mutex_lock (mutex);
01511
01512
            calibrate_best (i, e);
            calibrate_save_variables (i, e);
01513
01514
            g_mutex_unlock (mutex);
01515 #if DEBUG
            fprintf (stderr, "calibrate_thread: i=%u e=%lg\n", i, e);
01516
01517 #endif
01518
01519 #if DEBUG
01520
       fprintf (stderr, "calibrate_thread: end\n");
01521 #endif
01522
       g_thread_exit (NULL);
01523
        return NULL;
01524 }
```

Here is the call graph for this function:



5.7.3.11 int input_open (char * filename)

Function to open the input file.

Parameters

filename Input data file name.

Returns

1 on success, 0 on error.

Definition at line 488 of file mpcotool.c.

```
00489 {
00490
        char buffer2[64];
00491
        char *buffert[MAX_NINPUTS] =
00492
          { NULL, NULL, NULL, NULL, NULL, NULL, NULL, NULL };
00493
        xmlDoc *doc;
       xmlNode *node, *child;
xmlChar *buffer;
00494
00495
00496
        char *msg;
00497
        int error_code;
00498
        unsigned int i;
00499
00500 #if DEBUG
00501
       fprintf (stderr, "input_open: start\n");
00502 #endif
00503
00504
        // Resetting input data
00505
        buffer = NULL;
       input_new ();
00506
00507
       // Parsing the input file
00508
00509 #if DEBUG
       fprintf (stderr, "input_open: parsing the input file %s\n", filename);
00510
00511 #endif
        doc = xmlParseFile (filename);
00512
00513
        if (!doc)
00514
            msg = gettext ("Unable to parse the input file");
00515
00516
            goto exit on error;
00517
00518
        \ensuremath{//} Getting the root node
00519
00520 #if DEBUG
       fprintf (stderr, "input_open: getting the root node\n");
00521
00522 #endif
00523
        node = xmlDocGetRootElement (doc);
00524
        if (xmlStrcmp (node->name, XML_CALIBRATE))
00525
00526
            msg = gettext ("Bad root XML node");
00527
            goto exit_on_error;
00528
```

```
// Getting results file names
00531
        input->result = (char *) xmlGetProp (node, XML_RESULT);
00532
           (!input->result)
        input->result = (char *) xmlStrdup (result_name);
input->variables = (char *) xmlGetProp (node, XML_VARIABLES);
00533
00534
00535
        if (!input->variables)
00536
          input->variables = (char *) xmlStrdup (variables_name);
00537
        // Opening simulator program name
00538
00539
        input->simulator = (char *) xmlGetProp (node, XML_SIMULATOR);
        if (!input->simulator)
00540
00541
         {
00542
            msg = gettext ("Bad simulator program");
00543
            goto exit_on_error;
00544
00545
        // Opening evaluator program name
00546
        input->evaluator = (char *) xmlGetProp (node, XML_EVALUATOR);
00547
00548
00549
        // Obtaining pseudo-random numbers generator seed
        if (!xmlHasProp (node, XML_SEED))
  input->seed = DEFAULT_RANDOM_SEED;
00550
00551
00552
        else
00553
00554
            input->seed = xml_node_get_uint (node, XML_SEED, &error_code);
00555
            if (error_code)
00556
00557
                msg = gettext ("Bad pseudo-random numbers generator seed");
00558
                goto exit_on_error;
              }
00559
00560
          }
00561
00562
        // Opening algorithm
00563
        buffer = xmlGetProp (node, XML_ALGORITHM);
00564
        if (!xmlStrcmp (buffer, XML_MONTE_CARLO))
00565
00566
             input->algorithm = ALGORITHM MONTE CARLO;
00567
00568
             // Obtaining simulations number
00569
             input->nsimulations
00570
               = xml_node_get_int (node, XML_NSIMULATIONS, &error_code);
00571
             if (error_code)
00572
              {
00573
                msg = gettext ("Bad simulations number");
00574
                goto exit_on_error;
00575
              }
00576
        else if (!xmlStrcmp (buffer, XML_SWEEP))
input->algorithm = ALGORITHM_SWEEP;
00577
00578
00579
        else if (!xmlStrcmp (buffer, XML_GENETIC))
00580
          {
00581
            input->algorithm = ALGORITHM_GENETIC;
00582
00583
             // Obtaining population
            if (xmlHasProp (node, XML_NPOPULATION))
00584
00585
              {
                 input->nsimulations
00587
                   = xml_node_get_uint (node, XML_NPOPULATION, &error_code);
00588
                 if (error_code || input->nsimulations < 3)</pre>
00589
                     msg = gettext ("Invalid population number");
00590
00591
                     goto exit_on_error;
00592
                   }
00593
            else
00594
00595
             {
00596
                msg = gettext ("No population number");
00597
                goto exit_on_error;
00598
00599
00600
             // Obtaining generations
00601
             if (xmlHasProp (node, XML_NGENERATIONS))
00602
00603
                 input->niterations
                   = xml_node_get_uint (node, XML_NGENERATIONS, &error_code);
00604
                 if (error_code || !input->niterations)
00605
00606
                  {
00607
                    msg = gettext ("Invalid generations number");
00608
                     goto exit_on_error;
                   }
00609
00610
              }
00611
            else
00612
              {
00613
                 msg = gettext ("No generations number");
00614
                 goto exit_on_error;
00615
00616
```

```
// Obtaining mutation probability
00618
             if (xmlHasProp (node, XML_MUTATION))
00619
00620
                 input->mutation_ratio
                 = xml_node_get_float (node, XML_MUTATION, &error_code);
if (error_code || input->mutation_ratio < 0.</pre>
00621
00622
00623
                     || input->mutation_ratio >= 1.)
00624
00625
                      msg = gettext ("Invalid mutation probability");
00626
                      goto exit_on_error;
                   }
00627
00628
               }
00629
             else
00630
              {
00631
                 msg = gettext ("No mutation probability");
00632
                 goto exit_on_error;
00633
00634
00635
             // Obtaining reproduction probability
00636
             if (xmlHasProp (node, XML_REPRODUCTION))
00637
00638
                 input->reproduction_ratio
                 = xml_node_get_float (node, XML_REPRODUCTION, &error_code);
if (error_code || input->reproduction_ratio < 0.</pre>
00639
00640
00641
                      || input->reproduction_ratio >= 1.0)
00642
00643
                      msg = gettext ("Invalid reproduction probability");
00644
                     goto exit_on_error;
                   }
00645
00646
               }
00647
             else
00648
              {
00649
                 msg = gettext ("No reproduction probability");
00650
                 goto exit_on_error;
00651
00652
00653
             // Obtaining adaptation probability
             if (xmlHasProp (node, XML_ADAPTATION))
00654
00655
               {
00656
                 input->adaptation_ratio
                 = xml_node_get_float (node, XML_ADAPTATION, &error_code);
if (error_code || input->adaptation_ratio < 0.</pre>
00657
00658
00659
                      || input->adaptation_ratio >= 1.)
00660
                     msg = gettext ("Invalid adaptation probability");
00661
00662
                      goto exit_on_error;
00663
00664
               }
             else
00665
00666
              {
00667
                 msg = gettext ("No adaptation probability");
00668
                 goto exit_on_error;
00669
00670
00671
             // Checking survivals
             i = input->mutation_ratio * input->nsimulations;
00672
             i += input->reproduction_ratio * input->
00673
00674
             i += input->adaptation_ratio * input->
      nsimulations;
00675
            if (i > input->nsimulations - 2)
00676
              {
00677
                 msg = gettext
00678
                   ("No enough survival entities to reproduce the population");
00679
                 goto exit_on_error;
               }
00680
00681
          }
00682
        else
00683
         {
00684
            msg = gettext ("Unknown algorithm");
00685
            goto exit_on_error;
00686
        xmlFree (buffer);
buffer = NULL;
00687
00688
00689
         if (input->algorithm == ALGORITHM_MONTE_CARLO
00690
00691
             || input->algorithm == ALGORITHM_SWEEP)
00692
00693
00694
             // Obtaining iterations number
00695
             input->niterations
00696
               = xml_node_get_uint (node, XML_NITERATIONS, &error_code);
00697
             if (error_code == 1)
00698
               input->niterations = 1;
00699
             else if (error_code)
00700
               {
00701
                 msg = gettext ("Bad iterations number");
```

```
goto exit_on_error;
00703
00704
00705
            // Obtaining best number
00706
            if (xmlHasProp (node, XML_NBEST))
00707
              {
                input->nbest = xml_node_get_uint (node,
00708
     XML_NBEST, &error_code);
00709
               if (error_code || !input->nbest)
00710
                    msg = gettext ("Invalid best number");
00711
00712
                    goto exit_on_error;
00713
                  }
00714
00715
            else
00716
              input->nbest = 1;
00717
00718
            // Obtaining tolerance
            if (xmlHasProp (node, XML_TOLERANCE))
00720
              {
00721
                input->tolerance
00722
                  = xml_node_get_float (node, XML_TOLERANCE, &error_code);
00723
                if (error_code || input->tolerance < 0.)</pre>
00724
                  {
00725
                    msq = gettext ("Invalid tolerance");
00726
                    goto exit_on_error;
00727
                  }
00728
00729
            else
00730
              input->tolerance = 0.:
00731
00732
            // Getting gradient method parameters
00733
            if (xmlHasProp (node, XML_NSTEPS))
00734
              {
00735
                input->nsteps = xml_node_get_uint (node,
     XML_NSTEPS, &error_code);
00736
               if (error_code || !input->nsteps)
00737
                 {
00738
                    msg = gettext ("Invalid steps number");
00739
                    goto exit_on_error;
00740
                buffer = xmlGetProp (node, XML_GRADIENT_METHOD);
if (!xmlStrcmp (buffer, XML_COORDINATES))
00741
00742
                  input->gradient_method =
00743
     GRADIENT_METHOD_COORDINATES;
00744
               else if (!xmlStrcmp (buffer, XML_RANDOM))
00745
                    input->gradient_method =
00746
     GRADIENT_METHOD_RANDOM;
                   input->nestimates
00748
                       = xml_node_get_uint (node, XML_NESTIMATES, &error_code);
00749
                     if (error_code || !input->nestimates)
00750
00751
                        msg = gettext ("Invalid estimates number");
00752
                        goto exit_on_error;
00753
                      }
00754
                  }
00755
                else
00756
                    msg = gettext ("Unknown method to estimate the gradient");
00757
00758
                    goto exit_on_error;
00759
00760
                xmlFree (buffer);
00761
                buffer = NULL;
00762
                if (xmlHasProp (node, XML_RELAXATION))
00763
                  {
00764
                     input->relaxation
                       = xml_node_get_float (node, XML_RELAXATION, &error_code);
00765
                     if (error_code || input->relaxation < 0.</pre>
00766
00767
                        || input->relaxation > 2.)
00768
00769
                        msg = gettext ("Invalid relaxation parameter");
00770
                        goto exit_on_error;
00771
00772
00773
00774
                  input->relaxation = DEFAULT_RELAXATION;
00775
00776
            else
00777
              input->nsteps = 0;
00778
00779
00780
        // Reading the experimental data
00781
        for (child = node->children; child; child = child->next)
00782
00783
            if (xmlStrcmp (child->name, XML_EXPERIMENT))
00784
              break:
```

```
00785 #if DEBUG
            fprintf (stderr, "input_open: nexperiments=%u\n", input->nexperiments);
00786
00787 #endif
           if (xmlHasProp (child, XML_NAME))
buffer = xmlGetProp (child, XML_NAME);
00788
00789
00790
            else
00791
             {
00792
                snprintf (buffer2, 64, "%s %u: %s",
00793
                         gettext ("Experiment"),
00794
                          input->nexperiments + 1, gettext ("no data file name"));
00795
                msg = buffer2;
00796
                goto exit_on_error;
00797
00798 #if DEBUG
00799
            fprintf (stderr, "input_open: experiment=%s\n", buffer);
00800 #endif
00801
            input->weight = g_realloc (input->weight,
00802
                                        (1 + input->nexperiments) * sizeof (double));
            if (xmlHasProp (child, XML_WEIGHT))
00803
00804
             {
00805
                input->weight[input->nexperiments]
00806
                  = xml_node_get_float (child, XML_WEIGHT, &error_code);
00807
                if (error_code)
00808
                  {
00809
                    snprintf (buffer2, 64, "%s %s: %s",
                              gettext ("Experiment"), buffer, gettext ("bad weight"));
00810
00811
                    msg = buffer2;
                    goto exit_on_error;
00812
00813
                  }
00814
             }
00815
            else
00816
              input->weight[input->nexperiments] = 1.;
00817 #if DEBUG
00818
            fprintf (stderr, "input_open: weight=%lg\n",
00819
                     input->weight[input->nexperiments]);
00820 #endif
           if (!input->nexperiments)
00821
             input->ninputs = 0;
00823 #if DEBUG
00824
            fprintf (stderr, "input_open: template[0]\n");
00825 #endif
           if (xmlHasProp (child, XML_TEMPLATE1))
00826
00827
00828
                input->template[0]
00829
                 = (char **) g_realloc (input->template[0],
00830
                                          (1 + input->nexperiments) * sizeof (char *));
00831
                buffert[0] = (char *) xmlGetProp (child, template[0]);
00832 #if DEBUG
                fprintf (stderr, "input_open: experiment=%u template1=%s\n",
00833
                         input->nexperiments, buffert[0]);
00834
00835 #endif
00836
               if (!input->nexperiments)
00837
                  ++input->ninputs;
00838 #if DEBUG
                fprintf (stderr, "input_open: ninputs=%u\n", input->ninputs);
00839
00840 #endif
00841
              }
00842
            else
00843
             {
                snprintf (buffer2, 64, "%s %s: %s",
00844
                          gettext ("Experiment"), buffer, gettext ("no template"));
00845
00846
                msq = buffer2;
00847
                goto exit_on_error;
00848
00849
            for (i = 1; i < MAX_NINPUTS; ++i)</pre>
00850
00851 #if DEBUG
                fprintf (stderr, "input open: template%u\n", i + 1);
00852
00853 #endif
                if (xmlHasProp (child, template[i]))
00855
00856
                    if (input->nexperiments && input->ninputs <= i)</pre>
00857
                        00858
00859
                                  buffer, gettext ("bad templates number"));
00860
00861
                        msg = buffer2;
00862
                        while (i-- > 0)
00863
                          xmlFree (buffert[i]);
00864
                        goto exit_on_error;
00865
00866
                    input->template[i] = (char **)
                      g_realloc (input->template[i],
00867
00868
                                  (1 + input->nexperiments) * sizeof (char *));
00869
                    buffert[i] = (char *) xmlGetProp (child, template[i]);
00870 #if DEBUG
00871
                    fprintf (stderr, "input open: experiment=%u template%u=%s\n",
```

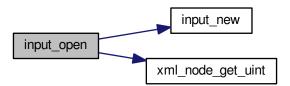
```
input->nexperiments, i + 1,
                              input->template[i][input->nexperiments]);
00873
00874 #endif
                   if (!input->nexperiments)
00875
                      ++input->ninputs;
00876
00877 #if DEBUG
                    fprintf (stderr, "input_open: ninputs=%u\n", input->ninputs);
00879 #endif
00880
00881
                else if (input->nexperiments && input->ninputs >= i)
00882
                    00883
00884
00885
                              buffer, gettext ("no template"), i + 1);
00886
                    msg = buffer2;
00887
                    while (i-- > 0)
                      xmlFree (buffert[i]);
00888
00889
                    goto exit_on_error;
00890
00891
                else
00892
00893
              1
            input->experiment
00894
              = g_realloc (input->experiment,
00895
00896
                           (1 + input->nexperiments) * sizeof (char *));
            input->experiment[input->nexperiments] = (char *) buffer;
00897
00898
            for (i = 0; i < input->ninputs; ++i)
00899
             input->template[i][input->nexperiments] = buffert[i];
00900
            ++input->nexperiments;
00901 #if DEBUG
            fprintf (stderr, "input_open: nexperiments=%u\n", input->nexperiments);
00902
00903 #endif
00904
00905
           (!input->nexperiments)
00906
            msq = gettext ("No calibration experiments");
00907
00908
            goto exit_on_error;
00910
        buffer = NULL:
00911
00912
        // Reading the variables data
00913
        for (; child; child = child->next)
00914
00915
            if (xmlStrcmp (child->name, XML_VARIABLE))
00916
00917
                snprintf (buffer2, 64, "%s %u: %s",
00918
                          gettext ("Variable"),
00919
                          input->nvariables + 1, gettext ("bad XML node"));
                msg = buffer2;
00920
00921
                goto exit_on_error;
00922
00923
            if (xmlHasProp (child, XML_NAME))
00924
             buffer = xmlGetProp (child, XML_NAME);
00925
            else
00926
              {
00927
                snprintf (buffer2, 64, "%s %u: %s",
                          gettext ("Variable"),
00928
00929
                           input->nvariables + 1, gettext ("no name"));
00930
                msg = buffer2;
00931
                goto exit_on_error;
00932
            if (xmlHasProp (child, XML_MINIMUM))
00933
00934
              {
00935
                input->rangemin = g_realloc
                (input->rangemin, (1 + input->nvariables) * sizeof (double));
input->rangeminabs = g_realloc
00936
00937
00938
                (input->rangeminabs, (1 + input->nvariables) * sizeof (double));
input->rangemin[input->nvariables]
00939
00940
                  = xml_node_get_float (child, XML_MINIMUM, &error_code);
00941
                if (error_code)
00942
                    snprintf (buffer2, 64, "%s %s: %s",
00943
                    gettext ("Variable"), buffer, gettext ("bad minimum"));
msg = buffer2;
00944
00945
00946
                    goto exit_on_error;
00947
00948
                if (xmlHasProp (child, XML_ABSOLUTE_MINIMUM))
00949
00950
                    input->rangeminabs[input->nvariables]
00951
                       = xml_node_get_float (child,
     XML_ABSOLUTE_MINIMUM, &error_code);
00952
                    if (error_code)
00953
                        snprintf (buffer2, 64, "%s %s: %s",
00954
                                   gettext ("Variable"),
00955
                                   buffer, gettext ("bad absolute minimum"));
00956
00957
                        msq = buffer2;
```

```
goto exit_on_error;
00959
00960
00961
                else
00962
                  input->rangeminabs[input->nvariables] = -G_MAXDOUBLE;
00963
                if (input->rangemin[input->nvariables]
                     < input->rangeminabs[input->nvariables])
00965
00966
                     snprintf (buffer2, 64, "%s %s: %s",
00967
                               gettext ("Variable"),
                              buffer, gettext ("minimum range not allowed"));
00968
00969
                    msq = buffer2;
00970
                    goto exit_on_error;
00971
00972
00973
            else
00974
00975
                snprintf (buffer2, 64, "%s %s: %s",
                           gettext ("Variable"), buffer, gettext ("no minimum range"));
                msg = buffer2;
00977
00978
                goto exit_on_error;
00979
            if (xmlHasProp (child, XML_MAXIMUM))
00980
00981
00982
                input->rangemax = q_realloc
                (input->rangemax, (1 + input->nvariables) * sizeof (double));
input->rangemaxabs = g_realloc
00983
00984
00985
                   (input->rangemaxabs, (1 + input->nvariables) * sizeof (double));
00986
                input->rangemax[input->nvariables]
00987
                  = xml_node_get_float (child, XML_MAXIMUM, &error_code);
00988
                if (error code)
00989
                  {
00990
                    snprintf (buffer2, 64, "%s %s: %s",
00991
                               gettext ("Variable"), buffer, gettext ("bad maximum"));
                    msg = buffer2;
00992
00993
                    goto exit_on_error;
00994
                if (xmlHasProp (child, XML_ABSOLUTE_MAXIMUM))
00996
                  {
00997
                     input->rangemaxabs[input->nvariables]
00998
                       = xml_node_get_float (child,
     XML_ABSOLUTE_MAXIMUM, &error_code);
00999
                    if (error_code)
01000
                        01001
01002
01003
                                   buffer, gettext ("bad absolute maximum"));
01004
                        msg = buffer2;
01005
                        goto exit_on_error;
01006
01007
01008
01009
                  input->rangemaxabs[input->nvariables] = G_MAXDOUBLE;
01010
                if (input->rangemax[input->nvariables]
                    > input->rangemaxabs[input->nvariables])
01011
                  {
01012
01013
                    snprintf (buffer2, 64, "%s %s: %s",
01014
                              gettext ("Variable"),
01015
                              buffer, gettext ("maximum range not allowed"));
                    msg = buffer2;
01016
01017
                    goto exit_on_error;
01018
01019
01020
            else
01021
01022
                snprintf (buffer2, 64, "%s %s: %s",
01023
                           gettext ("Variable"), buffer, gettext ("no maximum range"));
                msg = buffer2;
01024
01025
                goto exit_on_error;
01027
            if (input->rangemax[input->nvariables]
01028
                < input->rangemin[input->nvariables])
01029
                snprintf (buffer2, 64, "%s %s: %s",
01030
                           gettext ("Variable"), buffer, gettext ("bad range"));
01031
01032
                msg = buffer2;
01033
                goto exit_on_error;
01034
01035
            input->precision = g_realloc
            input->precision = g_learnor
  (input->precision, (1 + input->nvariables) * sizeof (unsigned int));
if (xmlHasProp (child, XML_PRECISION))
01036
01037
                input->precision[input->nvariables]
01039
01040
                   = xml_node_get_uint (child, XML_PRECISION, &error_code);
                if (error_code || input->precision[input->
01041
      nvariables] >= NPRECISIONS)
01042
                  {
```

```
snprintf (buffer2, 64, "%s %s: %s",
                             gettext ("Variable"),
01044
01045
                             buffer, gettext ("bad precision"));
                   msq = buffer2;
01046
01047
                   goto exit_on_error;
01048
01050
01051
             input->precision[input->nvariables] =
     DEFAULT PRECISION;
01052
           if (input->algorithm == ALGORITHM_SWEEP)
01053
             {
01054
               if (xmlHasProp (child, XML_NSWEEPS))
01055
01056
                   input->nsweeps = (unsigned int *)
01057
                    g_realloc (input->nsweeps,
                                (1 + input->nvariables) * sizeof (unsigned int));
01058
01059
                   input->nsweeps[input->nvariables]
                     = xml_node_get_uint (child, XML_NSWEEPS, &error_code);
01060
                   if (error_code || !input->nsweeps[input->
     nvariables])
01062
                       01063
01064
                                 buffer, gettext ("bad sweeps"));
01065
                      msg = buffer2;
01066
                       goto exit_on_error;
01067
01068
01069
                 }
01070
               else
01071
                {
01072
                   snprintf (buffer2, 64, "%s %s: %s",
01073
                            gettext ("Variable"),
01074
                             buffer, gettext ("no sweeps number"));
01075
                   msg = buffer2;
01076
                   goto exit_on_error;
01077
        fprintf (stderr, "input_open: nsweeps=%u nsimulations=%u\n",
                        input->nsweeps[input->nvariables],
01080
     input->nsimulations);
01081 #endif
01082
01083
           if (input->algorithm == ALGORITHM_GENETIC)
01084
01085
               // Obtaining bits representing each variable
01086
               if (xmlHasProp (child, XML_NBITS))
01087
                   input->nbits = (unsigned int *)
01088
                    g_realloc (input->nbits,
01089
                               (1 + input->nvariables) * sizeof (unsigned int));
01091
                   i = xml_node_get_uint (child, XML_NBITS, &error_code);
01092
                   if (error_code || !i)
01093
                     {
                       01094
01095
                                 buffer, gettext ("invalid bits number"));
01096
01097
                       msg = buffer2;
01098
                      goto exit_on_error;
01099
01100
                   input->nbits[input->nvariables] = i;
01101
01102
               else
01103
                   snprintf (buffer2, 64, "%s %s: %s",
01104
01105
                             gettext ("Variable"),
01106
                             buffer, gettext ("no bits number"));
                   msq = buffer2;
01107
01108
                   goto exit on error;
01109
01110
01111
           else if (input->nsteps)
01112
               input->step = (double *)
01113
                 g_realloc (input->step, (1 + input->nvariables) * sizeof (double));
01114
01115
               input->step[input->nvariables]
01116
                 = xml_node_get_float (child, XML_STEP, &error_code);
01117
               if (error_code || input->step[input->nvariables] < 0.)</pre>
01118
                  01119
01120
                             buffer, gettext ("bad step size"));
                   msg = buffer2;
01122
01123
                   goto exit_on_error;
01124
01125
01126
           input->label = g realloc
```

```
(input->label, (1 + input->nvariables) * sizeof (char *));
01128
            input->label[input->nvariables] = (char *) buffer;
01129
            ++input->nvariables;
01130
        if (!input->nvariables)
01131
01132
         {
01133
           msg = gettext ("No calibration variables");
01134
            goto exit_on_error;
01135
01136
       buffer = NULL;
01137
01138
       // Getting the working directory
        input->directory = g_path_get_dirname (filename);
01139
01140
       input->name = g_path_get_basename (filename);
01141
01142
       // Closing the XML document
01143
       xmlFreeDoc (doc);
01144
01145 #if DEBUG
01146
       fprintf (stderr, "input_open: end\n");
01147 #endif
01148
       return 1;
01149
01150 exit_on_error:
01151 xmlFree (buffer);
01152 xmlFreeDoc (doc);
01153
       show_error (msg);
01154 input_free ();
01155 #if DEBUG
01156
       fprintf (stderr, "input_open: end\n");
01157 #endif
01158
       return 0;
01159 }
```

Here is the call graph for this function:



5.7.3.12 void show_error (char * msg)

Function to show a dialog with an error message.

Parameters

```
msg Error message.
```

Definition at line 256 of file mpcotool.c.

```
00257 {
00258     show_message (gettext ("ERROR!"), msg, ERROR_TYPE);
00259 }
```

Here is the call graph for this function:



5.7.3.13 void show_message (char * title, char * msg, int type)

Function to show a dialog with a message.

Parameters

title	Title.
msg	Message.
type	Message type.

Definition at line 226 of file mpcotool.c.

```
00227 {
00228 #if HAVE_GTK
        GtkMessageDialog *dlg;
00230
00231
         // Creating the dialog
00232
        dlg = (GtkMessageDialog *) gtk_message_dialog_new
  (window->window, GTK_DIALOG_MODAL, type, GTK_BUTTONS_OK, "%s", msg);
00233
00234
00235
         // Setting the dialog title
00236
        gtk_window_set_title (GTK_WINDOW (dlg), title);
00237
        // Showing the dialog and waiting response
gtk_dialog_run (GTK_DIALOG (dlg));
00238
00239
00240
00241
         // Closing and freeing memory
00242
        gtk_widget_destroy (GTK_WIDGET (dlg));
00243
00245 printf ("%s: %s\n", title, msg);
00246 #endif
00247 }
```

5.7.3.14 double xml_node_get_float (xmlNode * node, const xmlChar * prop, int * error_code)

Function to get a floating point number of a XML node property.

Parameters

node	XML node.
prop	XML property.
error_code	Error code.

Returns

Floating point number value.

Definition at line 336 of file mpcotool.c.

00337 {

```
00338
       double x = 0.;
       xmlChar *buffer;
buffer = xmlGetProp (node, prop);
00340
       if (!buffer)
00341
00342
         *error_code = 1;
00343
       else
00345
        *e
else
*e
           if (sscanf ((char *) buffer, "%lf", &x) != 1)
00346
              *error_code = 2;
00347
00348
        xmlFree (buffer);
}
              *error_code = 0;
00349
00350
00351 return x;
00352 }
```

5.7.3.15 int xml_node_get_int (xmlNode * node, const xmlChar * prop, int * error_code)

Function to get an integer number of a XML node property.

Parameters

node	XML node.
prop	XML property.
error_code	Error code.

Returns

Integer number value.

Definition at line 274 of file mpcotool.c.

```
00275 {
00276
        int i = 0;
00277 xmlChar *buffer;
00278 buffer = xmlGetProp (node, prop);
00279
        if (!buffer)
00280
          *error_code = 1;
00281
        else
        {
  if (sscanf ((char *) buffer, "%d", &i) != 1)
  *error_code = 2;
00282
00283
00284
               *error_code = 2;
00285
           else
00286
              *error_code = 0;
00287
            xmlFree (buffer);
00288
00289
        return i;
00290 }
```

5.7.3.16 unsigned int xml_node_get_uint (xmlNode * node, const xmlChar * prop, int * error_code)

Function to get an unsigned integer number of a XML node property.

Parameters

node	XML node.
prop	XML property.
error_code	Error code.

Returns

Unsigned integer number value.

Definition at line 305 of file mpcotool.c.

```
00306 {
00307
        unsigned int i = 0;
       xmlChar *buffer;
buffer = xmlGetProp (node, prop);
00308
00309
        if (!buffer)
00310
00311
          *error_code = 1;
00312
        else
        {
00313
00314
            if (sscanf ((char *) buffer, "%u", &i) != 1)
00315
              *error_code = 2;
            else
00316
            *error_code = 0;
xmlFree (buffer);
00317
00318
00319
00320
       return i;
00321 }
```

5.7.3.17 void xml_node_set_float (xmlNode * node, const xmlChar * prop, double value)

Function to set a floating point number in a XML node property.

Parameters

node	XML node.
prop	XML property.
value	Floating point number value.

Definition at line 403 of file mpcotool.c.

5.7.3.18 void xml_node_set_int (xmlNode * node, const xmlChar * prop, int value)

Function to set an integer number in a XML node property.

Parameters

node	XML node.
prop	XML property.
value	Integer number value.

Definition at line 365 of file mpcotool.c.

5.7.3.19 void xml_node_set_uint (xmlNode * node, const xmlChar * prop, unsigned int value)

Function to set an unsigned integer number in a XML node property.

Parameters

node	XML node.
------	-----------

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prop	XML property.
value	Unsigned integer number value.

Definition at line 384 of file mpcotool.c.

5.8 mpcotool.h

```
00001 /*
00002 MPCOTool: a software to make calibrations of empirical parameters.
00003
00004 AUTHORS: Javier Burguete and Borja Latorre.
00006 Copyright 2012-2015, AUTHORS.
00007
00008 Redistribution and use in source and binary forms, with or without modification,
00009 are permitted provided that the following conditions are \operatorname{met}:
00010
00011
          1. Redistributions of source code must retain the above copyright notice,
00012
               this list of conditions and the following disclaimer.
00013
          Redistributions in binary form must reproduce the above copyright notice,
this list of conditions and the following disclaimer in the
00014
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               documentation and/or other materials provided with the distribution.
00017
00018 THIS SOFTWARE IS PROVIDED BY AUTHORS "AS IS" AND ANY EXPRESS OR IMPLIED
00019 WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF
00020 MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT
00021 SHALL AUTHORS OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, 00022 SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO,
00023 PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR
00024 BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN
00025 CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING
00026 IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY
00027 OF SUCH DAMAGE.
00028 */
00029
00036 #ifndef CALIBRATOR__H
00037 #define CALIBRATOR__H 1
00038
00043 enum Algorithm
00044 {
00045
        ALGORITHM_MONTE_CARLO = 0,
00046
        ALGORITHM_SWEEP = 1,
00047
        ALGORITHM_GENETIC =
00048 };
00049
00054 enum GradientMethod
00055 {
00056
        GRADIENT_METHOD_COORDINATES = 0,
00057
        GRADIENT_METHOD_RANDOM = 1,
00058 };
00059
00064 typedef struct
00065 {
00066
        char **template[MAX_NINPUTS];
00067
        char **experiment;
00068
        char **label;
00069
        char *result;
00070
        char *variables;
00071
        char *simulator:
00072
        char *evaluator;
        char *directory;
00074
00075
        char *name;
00076
        double *rangemin;
00077
        double *rangemax;
00078
        double *rangeminabs;
00079
        double *rangemaxabs;
08000
        double *weight;
00081
        double *step;
00082
        unsigned int *precision;
00083
        unsigned int *nsweeps;
00084
        unsigned int *nbits;
00086
        double tolerance:
00087
        double mutation_ratio;
00088
        double reproduction_ratio;
```

```
double adaptation_ratio;
00090
        double relaxation;
00091
        unsigned long int seed;
00093
        unsigned int nvariables;
00094
       unsigned int nexperiments;
00095
        unsigned int ninputs;
00096
        unsigned int nsimulations;
00097
        unsigned int algorithm;
00098
        unsigned int nsteps;
00100
       unsigned int gradient method;
00101
        unsigned int nestimates;
00103
       unsigned int niterations;
00104
        unsigned int nbest;
00105 } Input;
00106
00111 typedef struct
00112 {
        GMappedFile **file[MAX_NINPUTS];
00113
        char **template[MAX_NINPUTS];
char **experiment;
00115
00116
        char **label;
00117
        gsl_rng *rng;
        GeneticVariable *genetic_variable;
00118
        FILE *file_result;
00120
00121
        FILE *file_variables;
00122
        char *result;
00123
        char *variables;
00124
        char *simulator;
00125
        char *evaluator;
        double *value;
00127
       double *rangemin;
00128
00129
        double *rangemax;
00130
        double *rangeminabs;
00131
        double *rangemaxabs;
00132
        double *error_best;
00133
       double *weight;
00134
       double *step;
00135
       double *gradient;
00136
       double *value_old;
00138
       double *error_old;
00140
       unsigned int *precision;
       unsigned int *nsweeps;
00141
       unsigned int *thread;
00142
00144
       unsigned int *thread_gradient;
00147
        unsigned int *simulation_best;
00148
       double tolerance;
00149
       double mutation_ratio;
00150
       double reproduction_ratio;
00151
       double adaptation_ratio;
00152
       double relaxation;
00153
       double calculation_time;
00154
       unsigned long int seed;
00156
       unsigned int nvariables;
00157
       unsigned int nexperiments;
00158
       unsigned int ninputs;
00159
       unsigned int nsimulations;
00160
       unsigned int gradient_method;
00161
       unsigned int nsteps;
00163
       unsigned int nestimates;
00165
       unsigned int algorithm;
00166
       unsigned int nstart;
00167
       unsigned int nend;
00168
       unsigned int nstart_gradient;
00170
       unsigned int nend_gradient;
00172
       unsigned int niterations;
00173
       unsigned int nbest;
00174
       unsigned int nsaveds;
00175 #if HAVE_MPI
00176 int mpi_rank;
00177 #endif
00178 } Calibrate;
00179
00184 typedef struct
00185 {
00186
       unsigned int thread;
00187 } ParallelData;
00188
00189 // Public functions
00190 void show_message (char *title, char *msg, int type);
00191 void show_error (char *msg);
00192 int xml_node_get_int (xmlNode * node, const xmlChar * prop, int *error_code);
00193 unsigned int xml_node_get_uint (xmlNode * node, const xmlChar * prop,
00194
                                        int *error_code);
00195 double xml_node_get_float (xmlNode * node, const xmlChar * prop,
00196 int *error_code);
00197 void xml_node_set_int (xmlNode * node, const xmlChar * prop, int value);
00198 void xml_node_set_uint (xmlNode * node, const xmlChar * prop,
```

5.8 mpcotool.h

```
unsigned int value);
00200 void xml_node_set_float (xmlNode * node, const xmlChar * prop, double value);
00201 void input_new ();
00202 void input_free ();
00203 int input_open (char *filename);
00204 void calibrate_input (unsigned int simulation, char *input,
                             GMappedFile * template);
00206 double calibrate_parse (unsigned int simulation, unsigned int experiment);
00207 void calibrate_print ();
00208 void calibrate_save_variables (unsigned int simulation, double error);
00209 void calibrate_best (unsigned int simulation, double value);
00210 void calibrate_sequential ();
00211 void *calibrate_thread (ParallelData * data);
00212 void calibrate_merge (unsigned int nsaveds, unsigned int *simulation_best,
00213
                             double *error_best);
00214 #if HAVE MPI
00215 void calibrate_synchronise ();
00216 #endif
00217 void calibrate_sweep ();
00218 void calibrate_MonteCarlo ();
00219 void calibrate_best_gradient (unsigned int simulation, double value);
00220 void calibrate_gradient_sequential ();
00221 void *calibrate_gradient_thread (ParallelData * data);
{\tt 00222~double~calibrate\_variable\_step\_gradient~(unsigned~int~variable);}
00223 void calibrate_step_gradient (unsigned int simulation);
00224 void calibrate_gradient ();
00225 double calibrate_genetic_objective (Entity * entity);
00226 void calibrate_genetic ();
00227 void calibrate_save_old ();
00228 void calibrate_merge_old ();
00229 void calibrate_refine ();
00230 void calibrate_step ();
00231 void calibrate_iterate ();
00232 void calibrate_open ();
00233
00234 #endif
```

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