AMICI

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1 About AMICI

AMICI provides a multilanguage (Python, C++, Matlab) interface for the SUNDIALS solvers CVODES (for ordinary differential equations) and IDAS (for algebraic differential equations). AMICI allows the user to read differential equation models specified as SBML and automatically compiles such models as .mex simulation files, C++ executables or python modules. In contrast to the SUNDIALSTB interface, all necessary functions are transformed into native C++ code, which allows for a significantly faster simulation. Beyond forward integration, the compiled simulation file also allows for forward sensitivity analysis, steady state sensitivity analysis and adjoint sensitivity analysis for likelihood based output functions.

The interface was designed to provide routines for efficient gradient computation in parameter estimation of biochemical reaction models but is also applicable to a wider range of differential equation constrained optimization problems.

Online documentation is available as `github-pages`.

Publications

`Fröhlich, F., Kaltenbacher, B., Theis, F. J., & Hasenauer, J. (2017). Scalable Parameter Estimation for Genome-Scale Biochemical Reaction Networks. Plos Computational Biology, 13(1), e1005331. doi: 10.1371/journal.pcbi.1005331`

`Fröhlich, F., Theis, F. J., Rädler, J. O., & Hasenauer, J. (2017). Parameter estimation for dynamical systems with discrete events and logical operations. Bioinformatics, 33(7), 1049-1056. doi: 10.1093/bioinformatics/btw764`

Current build status

2 License Conditions

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3 How to contribute

We are happy about contributions to AMICI in any form (new functionality, documentation, bug reports, ...).

Making code changes

When making code changes:

- Check if you agree to release your contribution under the conditions provided in `LICENSE`
- Start a new branch from `develop`
- Implement your changes
- Submit a pull request to the `develop` branch
- Make sure your code is documented appropriately
  - Run `mtoc/makeDocumentation.m` to check completeness of your documentation
- Make sure your code is compatible with C++11, `gcc` and `clang`
- when adding new functionality, please also provide test cases (see `tests/cpputest/`)
- Write meaningful commit messages
- Run all tests to ensure nothing was broken
  - Run `tests/cpputest/wrapTestModels.m` followed by CI tests `scripts/buildAll.sh && scripts/run-cpputest.sh`
  - Run `tests/testModels.m`
  - Run `make python-tests` in `build`
- When all tests are passing and you think your code is ready to merge, request a code review

Adding/Updating tests

To add new tests add a new corresponding python script (see, e.g., `tests/example_dirac.py`) and add it to and run `tests/generateTestConfigurationForExamples.sh` To update test results replace `tests/cpputest/expectedResults.h5` by `tests/cpputest/writeResults.h5.bak` [ONLY DO THIS AFTER TRIPLE CHECKING CORRECTNESS OF RESULTS] Before replacing the test results, confirm that only expected datasets have changed, e.g. using `h5diff -v -r 1e-8 tests/cpputest/expectedResults.h5 tests/cpputest/writeResults.h5.bak | less`

4 Installation

Availability

The sources for AMICI are accessible as

- Source `tarball`
- Source `zip`
- GIT repository on `github`

Obtaining AMICI via the GIT versioning system

In order to always stay up-to-date with the latest AMICI versions, simply pull it from our GIT repository and recompile it when a new release is available. For more information about GIT checkout their website

The GIT repository can currently be found at https://github.com/ICB-DCM/AMICI and a direct clone is possible via

```
git clone https://github.com/ICB-DCM/AMICI.git AMICI
```

Installation

If AMICI was downloaded as a zip, it needs to be unpacked in a convenient directory. If AMICI was obtained via cloning of the git repository, no further unpacking is necessary.

Dependencies

The MATLAB interface only depends on the symbolic toolbox, which is needed for model compilation, but not simulation.

Symbolic Engine

The MATLAB interface requires the symbolic toolbox for model compilation. The symbolic toolbox is not required for model simulation.

Math Kernel Library (MKL)

The python and C++ interfaces require a system installation of BLAS. AMICI has been tested with various native and general purpose MKL implementations such as Accelerate, Intel MKL, cblas, openblas, atlas. The matlab interface uses the MATLAB MKL, which requires no prior installation.

HDF5

The python and C++ interfaces provide routines to read and write options and results in hdf5 format. For the python interface, the installation of hdf5 is optional, but for the C++ interace it is required. HDF can be installed using package managers such as brew or apt:

```
brew install hdf5
```

or

```
apt-get install libhdf5-serial-dev
```

SWIG

The python interface requires SWIG, which has to be installed by the user. Swig can be installed using package managers such as brew or apt:

```
brew install swig
```

or

```
apt-get install swig3.0
```

We note here that some linux package managers may provide swig executables as swig3.0, but installation as swig is required. This can be fixed using, e.g., symbolic links:

```
mkdir -p ~/bin/ && ln -s $(which swig3.0) ~/bin/swig && export PATH=~/bin/:$PATH
```

python packages

The python interface requires the python packages `pkgconfig` and `numpy` to be installed before AMICI can be installed. These can be installed via `pip`:

```
pip3 install pkgconfig numpy
```

MATLAB

To use AMICI from MATLAB, start MATLAB and add the AMICI/matlab direcory to the MATLAB path. To add all toolbox directories to the MATLAB path, execute the matlab script

```
installAMICI.m
```

To store the installation for further MATLAB session, the path can be saved via

```
savepath
```

For the compilation of .mex files, MATLAB needs to be configured with a working C compiler. The C compiler needs to be installed and configured via:

```
mex -setup c
```

For a list of supported compilers we refer to the mathworks documentation: `mathworks.com` Note that Microsoft Visual Studio compilers are currently not supported.

python

To use AMICI from python, install the module and all other requirements using pip

```
pip3 install amici
```

You can now import it as python module:

```
import amici
```

C++

To use AMICI from C++, run the

```
./scripts/buildSundials.sh
./scripts/buildSuitesparse.sh
./scripts/buildAmici.sh
```

script to compile amici libary. The static library file can then be linked from

```
./build/libamici.a
```

In CMake-based packages, amici can be linked via

```
find_package(Amici)
```

Dependencies

The MATLAB interface requires the Mathworks Symbolic Toolbox for model generation via `amiwrap(...)`, but not for execution of precompiled models. Currently MATLAB R2018a or newer is not supported (see https://github.com/ICB-DCM/AMICI/issues/307)

The python interface requires python 3.6 or newer and `cblas` library to be installed. Windows installations via pip are currently not supported, but users may try to install amici using the build scripts provided for the C++ interface (these will by default automatically install the python module).

The C++ interface requires `cmake` and `cblas` to be installed.

The tools SUNDIALS and SuiteSparse shipped with AMICI do **not** require explicit installation.

AMICI uses the following packages from SUNDIALS:

CVODES: the sensitivity-enabled ODE solver in SUNDIALS. Radu Serban and Alan C. Hindmarsh. *ASME 2005 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference.* American Society of Mechanical Engineers, 2005. PDF

IDAS

AMICI uses the following packages from SuiteSparse:

Algorithm 907: KLU, A Direct Sparse Solver for Circuit Simulation Problems. Timothy A. Davis, Ekanathan Palamadai Natarajan, *ACM Transactions on Mathematical Software*, Vol 37, Issue 6, 2010, pp 36:1 - 36:17. PDF

Algorithm 837: AMD, an approximate minimum degree ordering algorithm, Patrick R. Amestoy, Timothy A. Davis, Iain S. Duff, *ACM Transactions on Mathematical Software*, Vol 30, Issue 3, 2004, pp 381 - 388. PDF

Algorithm 836: COLAMD, a column approximate minimum degree ordering algorithm, Timothy A. Davis, John R. Gilbert, Stefan I. Larimore, Esmond G. Ng *ACM Transactions on Mathematical Software*, Vol 30, Issue 3, 2004, pp 377 - 380. PDF

5 Python Interface

In the following we will give a detailed overview how to specify models in Python and how to call the generated simulation files.

Model Definition

This guide will guide the user on how to specify models in Python using SBML. For example implementations see the examples in the python/examples directory.

SBML input

First, import an sbml file using the `amici.sbml_import.SbmlImporter` class:

```
import amici
sbmlImporter = amici.SbmlImporter('model_steadystate_scaled.sbml')
```

the sbml document as imported by `libSBML` is available as

```
sbml = sbmlImporter.sbml
```

Constants

parameters that should be considered constants can be specified in a list of strings specifying the respective SbmlId of a parameter.

```
constantParameters=['k4']
```

Observables

assignment rules that should be considered as observables can extracted using the `amici.assignment↩Rules2observables` function

```
observables = amici.assignmentRules2observables(sbml, filter=lambda variableId:
                                                variableId.startswith('observable_') and not variableId.endswi
```

Standard Deviations

standard deviations can be specified as dictionaries ...

```
sigmas = {'observable_x1withsigma': 'observable_x1withsigma_sigma'}
```

Model Compilation

to compile the sbml as python module, the user has to call the method `amici.sbml_import.SbmlImporter.sbml2amici`, passing all the previously defined model specifications

```
sbmlImporter.sbml2amici('test', 'test',
                        observables=observables,
                        constantParameters=constantParameters,
                        sigmas=sigma)
```

Note: To build AMICI with OpenMP support, which allows to parallelize model simulations of multiple experimental conditions, set the environment variables `AMICI_CXXFLAGS` and `AMICI_LDFLAGS` to the correct OpenMP flags of your compiler and linker, respectively. This has to be done for both AMICI package installation *and* model compilation. When using `gcc` on Linux, use:

```
# on your shell:
AMICI_CXXFLAGS=-fopenmp AMICI_LDFLAGS=-fopenmp pip3 install amici

# in python, before model compilation:
import os
os.environ['AMICI_CXXFLAGS'] = '-fopenmp'
os.environ['AMICI_LDFLAGS'] = '-fopenmp'
```

Model Simulation

currently the model folder has to be manually added to the python path

```
import sys
sys.path.insert(0, 'test')
```

the compiled model can now be imported as python module

```
import test as modelModule
```

to obtain a model instance call the `getModel()` method. This model instance will be instantiated using the defautl parameter values specified in the sbml.

```
model = modelModule.getModel()
```

then pass the simulation timepoints to `amici.Model.setTimepoints`

```
model.setTimepoints(np.linspace(0, 60, 60))
```

for simulation we need to generate a solver instance

```
solver = model.getSolver()
```

the model simulation can now be carried out using `amici.runAmiciSimulation`

```
rdata = amici.runAmiciSimulation(model, solver)
```

6 MATLAB Interface

In the following we will give a detailed overview how to specify models in MATLAB and how to call the generated simulation files.

Model Definition

This guide will guide the user on how to specify models in MATLAB. For example implementations see the examples in the matlab/examples directory.

Header

The model definition needs to be defined as a function which returns a struct with all symbolic definitions and options.

```
function [model] = example_model_syms()
```

Options

Set the options by specifying the respective field of the modelstruct

```
model.(fieldname) = value
```

The options specify default options for simulation, parametrisation and compilation. All of these options are optional.

field	description	default
.param	default parametrisation 'log'/'log10'/'lin'	'lin'
.debug	flag to compile with debug symbols	false
.forward	flag to activate forward sensitivities	true
.adjoint	flag to activate adjoint sensitivities	true

When set to false, the fields 'forward' and 'adjoint' will speed up the time required to compile the model but also disable the respective sensitivity computation.

States

Create the respective symbolic variables. The name of the symbolic variable can be chosen arbitrarily.

```
syms state1 state2 state3
```

Create the state vector containing all states:

```
model.sym.x = [ state1 state2 state3 ];
```

Parameters

Create the respective symbolic variables. The name of the symbolic variable can be chosen arbitrarily. Sensitivities **will be derived** for all paramaters.

```
syms param1 param2 param3 param4 param5 param6
```

Create the parameters vector

```
model.sym.p = [ param1 param2 param3 param4 param5 param6 ];
```

Constants

Create the respective symbolic variables. The name of the symbolic variable can be chosen arbitrarily. Sensitivities with respect to constants **will not be derived**.

```
syms const1 const2
```

Create the parameters vector

```
model.sym.k = [ const1 const2 ];
```

Differential Equation

For time-dependent differential equations you can specify a symbolic variable for time. This **needs** to be denoted by `t`.

```
syms t
```

Specify the right hand side of the differential equation `f` or `xdot`

```
model.sym.xdot(1) = [ const1 - param1*state1 ];
model.sym.xdot(2) = [ +param2*state1 + dirac(t-param3) - const2*state2 ];
model.sym.xdot(3) = [ param4*state2 ];
```

or

```
model.sym.f(1) = [ const1 - param1*state1 ];
model.sym.f(2) = [ +param2*state1 + dirac(t-param3) - const2*state2 ];
model.sym.f(3) = [ param4*state2 ];
```

The specification of `f` or `xdot` may depend on states, parameters and constants.

For DAEs also specify the mass matrix.

```
model.sym.M = [1, 0, 0;...
               0, 1, 0;...
               0, 0, 0];
```

The specification of M may depend on parameters and constants.

For ODEs the integrator will solve the equation $\dot{x} = f$ and for DAEs the equations $M \cdot \dot{x} = f$. AMICI will decide whether to use CVODES (for ODEs) or IDAS (for DAEs) based on whether the mass matrix is defined or not.

In the definition of the differential equation you can use certain symbolic functions. For a full list of available functions see `src/symbolic_functions.cpp`.

Dirac functions can be used to cause a jump in the respective states at the specified time-point. This is typically used to model injections, or other external stimuli. Spline functions can be used to model time/state dependent response with unkown time/state dependence.

Initial Conditions

Specify the initial conditions. These may depend on parameters on constants and must have the same size as `x`.

```
model.sym.x0 = [ param4, 0, 0 ];
```

Observables

Specify the observables. These may depend on parameters and constants.

```
model.sym.y(1) = state1 + state2;
model.sym.y(2) = state3 - state2;
```

In the definition of the observable you can use certain symbolic functions. For a full list of available functions see `src/symbolic_functions.cpp`. Dirac functions in observables will have no effect.

Events

Specifying events is optional. Events are specified in terms of a trigger function, a bolus fuction and an output function. The roots of the trigger function defines the occurences of the event. The bolus function defines the change in the state on event occurences. The output function defines the expression which is evaluated and reported by the simulation routine on every event occurence. The user can create events by constructing a vector of objects of the class amievent.

```
model.sym.event(1) = amievent(state1 - state2,0,[]);
```

Events may depend on states, parameters and constants but **not** on observables.

For more details about event support see https://doi.org/10.1093/bioinformatics/btw764

Standard Deviation

Specifying standard deviations is optional. It only has an effect when computing adjoint sensitivities. It allows the user to specify standard deviations of experimental data for observables and events.

Standard deviaton for observable data is denoted by sigma_y

```
model.sym.sigma_y(1) = param5;
```

Standard deviaton for event data is denoted by sigma_t

```
model.sym.sigma_t(1) = param6;
```

Both `sigma_y` and `sigma_t` can either be a scalar or of the same dimension as the observables / events function. They can depend on time and parameters but must not depend on the states or observables. The values provided in `sigma_y` and `sigma_t` will only be used if the value in `D.Sigma_Y` or `D.Sigma_T` in the user-provided data struct is `NaN`. See simulation for details.

Objective Function

By default, AMICI assumes a normal noise model and uses the corresponding negative log-likelihood

```
J = 1/2*sum(((y_i(t)-my_ti)/sigma_y_i)^2 + log(2*pi*sigma_y^2)
```

as objective function. A user provided objective function can be specified in

```
model.sym.Jy
```

As reference see the default specification of `this.sym.Jy` in `amimodel.makeSyms`.

SBML

AMICI can also import SBML models using the command `SBML2AMICI`. This will generate a model specification as described above, which may be edited by the user to apply further changes.

Model Compilation

The model can then be compiled by calling `amiwrap.m`:

```
amiwrap(modelname,'example_model_syms',dir,o2flag)
```

Here `modelname` should be a string defining the name of the model, `dir` should be a string containing the path to the directory in which simulation files should be placed and `o2flag` is a flag indicating whether second order sensitivities should also be compiled. The user should make sure that the previously defined function ''example_model_syms'`is in the user path. Alternatively, the user can also call the function`'example_model_syms''

```
[model] = example_model_syms()
```

and subsequently provide the generated struct to `amiwrap(...)`, instead of providing the symbolic function:

```
amiwrap(modelname,model,dir,o2flag)
```

In a similar fashion, the user could also generate multiple models and pass them directly to `amiwrap(...)` without generating respective model definition scripts.

Model Simulation

After the call to `amiwrap(...)` two files will be placed in the specified directory. One is a *modelname*.mex and the other is simulate_ *modelname*.m. The mex file should never be called directly. Instead the MATLAB script, which acts as a wrapper around the .mex simulation file should be used.

The simulate_ *modelname*.m itself carries extensive documentation on how to call the function, what it returns and what additional options can be specified. In the following we will give a short overview of possible function calls.

Integration

Define a time vector:

```
t = linspace(0,10,100)
```

Generate a parameter vector:

```
theta = ones(6,1);
```

Generate a constants vector:

```
kappa = ones(2,1);
```

Integrate:

```
sol = simulate_modelname(t,theta,kappa,[],options)
```

The integration status will be indicated by the `sol.status` flag. Negative values indicated failed integration. The states will then be available as sol.x. The observables will then be available as `sol.y`. The event outputs will then be available as `sol.z`. If no event occured there will be an event at the end of the considered interval with the final value of the root function is stored in `sol.rz`.

Alternatively the integration can also be called via

```
[status,t,x,y] = simulate_modelname(t,theta,kappa,[],options)
```

The integration status will be indicated by the flag `status` . Negative values indicated failed integration. The states will then be available as `x`. The observables will then be available as `y`. No event output will be given.

Forward Sensitivities

Set the sensitivity computation to forward sensitivities and integrate:

```
options.sensi = 1;
options.sensi_meth = 'forward;
sol = simulate_modelname(t,theta,kappa,[],options)
```

The integration status will be indicated by the `sol.status` flag. Negative values indicate failed integration. The states will be available as `sol.x`, with the derivative with respect to the parameters in `sol.sx`. The observables will be available as `sol.y`, with the derivative with respect to the parameters in `sol.sy`. The event outputs will be available as `sol.z`, with the derivative with respect to the parameters in `sol.sz`. If no event occured there will be an event at the end of the considered interval with the final value of the root function stored in `sol.rz`, with the derivative with respect to the parameters in `sol.srz`.

Alternatively the integration can also be called via

```
[status,t,x,y,sx,sy] = simulate_modelname(t,theta,kappa,[],options)
```

The integration status will be indicated by the status flag. Negative values indicate failed integration. The states will then be available as `x`, with derivative with respect to the parameters in `sx`. The observables will then be available as `y`, with derivative with respect to the parameters in `sy`. No event output will be given.

Adjoint Sensitivities

Set the sensitivity computation to adjoint sensitivities:

```
options.sensi = 1;
options.sensi_meth = 'adjoint';
```

Define Experimental Data:

```
D.Y = [NaN(1,2)],ones(length(t)-1,2)];
D.Sigma_Y = [0.1*ones(length(t)-1,2),NaN(1,2)];
D.T = ones(1,1);
D.Sigma_T = NaN;
```

The `NaN` values in `Sigma_Y` and `Sigma_T` will be replaced by the specification in `model.sym.sigma_y` and `model.sym.sigma_t`. Data points with `NaN` value will be completely ignored.

Integrate:

```
sol = simulate_modelname(t,theta,kappa,D,options)
```

The integration status will be indicated by the sol.status flag. Negative values indicate failed integration. The log-likelihood will then be available as `sol.llh` and the derivative with respect to the parameters in `sol.sllh`. Notice that for adjoint sensitivities no state, observable and event sensitivities will be available. Yet this approach can be expected to be significantly faster for systems with a large number of parameters.

Steady State Sensitivities

This will compute state sensitivities according to the formula $s_k^x = -\left(\frac{\partial f}{\partial x}\right)^{-1} \frac{\partial f}{\partial \theta_k}$

In the current implementation this formulation does not allow for conservation laws as this would result in a singular Jacobian.

Set the final timepoint as infinity, this will indicate the solver to compute the steadystate:

```
t = Inf;
```

Set the sensitivity computation to steady state sensitivities:

```
options.sensi = 1;
```

Integrate:

```
sol = simulate_modelname(t,theta,kappa,D,options)
```

The states will be available as `sol.x`, with the derivative with respect to the parameters in `sol.sx`. The observables will be available as `sol.y`, with the derivative with respect to the parameters in `sol.sy`. Notice that for steady state sensitivities no event sensitivities will be available. For the accuracy of the computed derivatives it is essential that the system is sufficiently close to a steady state. This can be checked by examining the right hand side of the system at the final time-point via `sol.diagnosis.xdot`.

7 C++ Interface

The Python Interface and MATLAB Interface can translate the model definition into C++ code, which is then compiled into a .mex file or a python module. Advanced users can also use this code within stand-alone C/C++ application for use in other environments (e.g. on high performance computing systems). This section will give a short overview over the generated files and provide a brief introduction of how this code can be included in other applications.

Generated model files

`amiwrap.m` and `amici.SbmlImporter.sbml2amici` write the model source files to ${AMICI_ROOT_↩ DIR}/models/${MODEL_NAME} by default. The content of a model source directory might look something like this (given `MODEL_NAME=model_steadystate`):

```
CMakeLists.txt
hashes.mat
main.cpp
model_steadystate_deltaqB.cpp
model_steadystate_deltaqB.h
[... many more files model_steadystate_*.(cpp|h|md5|o) ]
wrapfunctions.cpp
wrapfunctions.h
model_steadystate.h
```

Running a simulation

The entry function for running an AMICI simulation is `runAmiciSimulation(...)`, declared in amici.h. This function requires (i) a `Model` instance. For the example `model_steadystate` the respective class is provided as `Model_model_steadystate` in `model_steadystate.h`. For convenience, the header `wrapfunctions.h` defines a function `getModel()`, that returns an instance of that class. (ii) a `Solver` instance. This solver instance needs to match the requirements of the model and can be generated using `model->getSolver()`. (iii) optionally an `ExpData` instance, which contains any experimental data.

A scaffold for a standalone simulation program is generated in `main.cpp` in the model source directory. This programm shows how to initialize the above-mentioned structs and how to obtain the simulation results.

Compiling and linking

The complete AMICI API is available through `amici.h`; this is the only header file that needs to be included. `hdf5.h` provides some functions for reading and writing `HDF5` files).

You need to compile and link `${AMICI_ROOT_DIR}/models/${MODEL_NAME}/*.cpp`, `${AMICI_ROOT_DIR}/src/*.cpp`, the SUNDIALS and the SUITESPARSE library, or use the CMake package configuration from the build directory which tells CMake about all AMICI dependencies.

Along with `main.cpp`, a `CMake` file (`CMakeLists.txt`) will be generated automatically. The CMake file shows the abovementioned library dependencies. These files provide a scaffold for a standalone simulation program. The required numerical libraries are shipped with AMICI. To compile them, run `${AMICI_ROOT_DIR}/scripts/run-tests.sh` once. HDF5 libraries and header files need to be installed separately. More information on how to run the compiled program is provided in `main.cpp`.

8 FAQ

Q: My model fails to build.

A: Remove the corresponding model directory located in AMICI/models/∗yourmodelname∗ and compile again.

Q: It still does not compile.

A: Make an `issue` and we will have a look.

Q: I get an out of memory error while compiling my model on a Windows machine.

A: This may be due to an old compiler version. See `issue #161` for instructions on how to install a new compiler.

Q: The simulation/sensitivities I get are incorrect.

A: There are some known issues, especially with adjoint sensitivities, events and DAEs. If your particular problem is not featured in the `issues` list, please add it!

9 Namespace Documentation

9.1 amici Namespace Reference

The AMICI Python module (in doxygen this will also contain documentation about the C++ library)

Namespaces

- ode_export

  The C++ ODE export module for python.
- plotting

  Plotting related functions.
- sbml_import

  The python sbml import module for python.

Classes

- class AmiException

  amici exception handler class
- class AmiVector
- class AmiVectorArray
- class BackwardProblem

  class to solve backwards problems.
- class CvodeException

  cvode exception handler class
- class ExpData

  ExpData carries all information about experimental or condition-specific data.
- class ForwardProblem

  The ForwardProblem class groups all functions for solving the backwards problem. Has only static members.
- class IDAException

  ida exception handler class
- class IntegrationFailure

  integration failure exception for the forward problem this exception should be thrown when an integration failure occured for this exception we can assume that we can recover from the exception and return a solution struct to the user
- class IntegrationFailureB

  integration failure exception for the backward problem this exception should be thrown when an integration failure occured for this exception we can assume that we can recover from the exception and return a solution struct to the user
- class Model

  The Model class represents an AMICI ODE model. The model can compute various model related quantities based on symbolically generated code.
- class Model_DAE

  The Model class represents an AMICI DAE model. The model does not contain any data, but represents the state of the model at a specific time t. The states must not always be in sync, but may be updated asynchroneously.
- class Model_ODE

  The Model class represents an AMICI ODE model. The model does not contain any data, but represents the state of the model at a specific time t. The states must not always be in sync, but may be updated asynchroneously.
- class NewtonFailure

  newton failure exception this exception should be thrown when the steady state computation failed to converge for this exception we can assume that we can recover from the exception and return a solution struct to the user
- class NewtonSolver

  The NewtonSolver class sets up the linear solver for the Newton method.
- class NewtonSolverDense

  The NewtonSolverDense provides access to the dense linear solver for the Newton method.
- class NewtonSolverIterative

  The NewtonSolverIterative provides access to the iterative linear solver for the Newton method.
- class NewtonSolverSparse

The NewtonSolverSparse provides access to the sparse linear solver for the Newton method.

- class ReturnData

  class that stores all data which is later returned by the mex function

- class SetupFailure

  setup failure exception this exception should be thrown when the solver setup failed for this exception we can assume that we cannot recover from the exception and an error will be thrown

- class Solver
- class SteadystateProblem

  The SteadystateProblem class solves a steady-state problem using Newton's method and falls back to integration on failure.

Typedefs

- typedef double realtype
- typedef void(∗ msgIdAndTxtFp) (const char ∗identifier, const char ∗format,...)

  msgIdAndTxtFp

Enumerations

- enum BLASLayout { **rowMajor** = 101, **colMajor** = 102 }
- enum BLASTranspose { **noTrans** = 111, **trans** = 112, **conjTrans** = 113 }
- enum ParameterScaling { **none**, **ln**, **log10** }
- enum SecondOrderMode { **none**, **full**, **directional** }
- enum SensitivityOrder { **none**, **first**, **second** }
- enum SensitivityMethod { **none**, **forward**, **adjoint** }
- enum LinearSolver {
  dense = 1, **band** = 2, **LAPACKDense** = 3, **LAPACKBand** = 4,
  diag = 5, **SPGMR** = 6, **SPBCG** = 7, **SPTFQMR** = 8,
  KLU = 9 }
- enum InternalSensitivityMethod { **simultaneous** = 1, **staggered** = 2, **staggered1** = 3 }
- enum InterpolationType { **hermite** = 1, **polynomial** = 2 }
- enum LinearMultistepMethod { **adams** = 1, **BDF** = 2 }
- enum NonlinearSolverIteration { **functional** = 1, **newton** = 2 }
- enum StateOrdering { **AMD**, **COLAMD**, **natural** }
- enum SteadyStateSensitivityMode { **newtonOnly**, **simulationFSA** }
- enum NewtonStatus { **failed** =-1, **newt** =1, **newt_sim** =2, **newt_sim_newt** =3 }
- enum mexRhsArguments {
  RHS_TIMEPOINTS, **RHS_PARAMETERS**, **RHS_CONSTANTS**, **RHS_OPTIONS**,
  RHS_PLIST, **RHS_XSCALE_UNUSED**, **RHS_INITIALIZATION**, **RHS_DATA**,
  RHS_NUMARGS_REQUIRED = RHS_DATA, **RHS_NUMARGS** }

  The mexFunctionArguments enum takes care of the ordering of mex file arguments (indexing in prhs)

Functions

- void printErrMsgIdAndTxt (const char ∗identifier, const char ∗format,...)
- void printWarnMsgIdAndTxt (const char ∗identifier, const char ∗format,...)
- std::unique_ptr< ReturnData > runAmiciSimulation (Solver &solver, const ExpData ∗edata, Model &model)
- std::vector< std::unique_ptr< ReturnData > > runAmiciSimulations (Solver const &solver, const std↩ ::vector< ExpData ∗> &edatas, Model const &model, int num_threads)
- void amici_dgemv (BLASLayout layout, BLASTranspose TransA, const int M, const int N, const double alpha, const double ∗A, const int lda, const double ∗X, const int incX, const double beta, double ∗Y, const int incY)

- void amici_dgemm (BLASLayout layout, BLASTranspose TransA, BLASTranspose TransB, const int M, const int N, const int K, const double alpha, const double ∗A, const int lda, const double ∗B, const int ldb, const double beta, double ∗C, const int ldc)
- void amici_daxpy (int n, double alpha, const double ∗x, const int incx, double ∗y, int incy)

  Compute y = a∗x + y.
- void setModelData (const mxArray ∗prhs[ ], int nrhs, Model &model)

  setModelData sets data from the matlab call to the model object
- void setSolverOptions (const mxArray ∗prhs[ ], int nrhs, Solver &solver)

  setSolverOptions solver options from the matlab call to a solver object
- ReturnDataMatlab ∗ setupReturnData (mxArray ∗plhs[ ], int nlhs)
- std::unique_ptr< ExpData > expDataFromMatlabCall (const mxArray ∗prhs[ ], const Model &model)
- int checkFinite (const int N, const realtype ∗array, const char ∗fun)
- void unscaleParameters (const double ∗bufferScaled, const ParameterScaling ∗pscale, int n, double ∗buffer↩ Unscaled)

  Remove parameter scaling according to the parameter scaling in pscale.
- void unscaleParameters (std::vector< double > const &bufferScaled, std::vector< ParameterScaling > const &pscale, std::vector< double > &bufferUnscaled)

  Remove parameter scaling according to the parameter scaling in pscale.
- double getUnscaledParameter (double scaledParameter, ParameterScaling scaling)

  Remove parameter scaling according to `scaling`
- double getScaledParameter (double unscaledParameter, ParameterScaling scaling)

  Apply parameter scaling according to `scaling`
- void scaleParameters (const std::vector< double > &bufferUnscaled, const std::vector< ParameterScaling > &pscale, std::vector< double > &bufferScaled)

  Apply parameter scaling according to `scaling`
- bool operator== (const Model &a, const Model &b)
- mxArray ∗ getReturnDataMatlabFromAmiciCall (ReturnData const ∗rdata)
- mxArray ∗ initMatlabReturnFields (ReturnData const ∗rdata)
- mxArray ∗ initMatlabDiagnosisFields (ReturnData const ∗rdata)
- template<typename T >
  void writeMatlabField0 (mxArray ∗matlabStruct, const char ∗fieldName, T fieldData)
- template<typename T >
  void writeMatlabField1 (mxArray ∗matlabStruct, const char ∗fieldName, std::vector< T > fieldData, const int dim0)
- template<typename T >
  void writeMatlabField2 (mxArray ∗matlabStruct, const char ∗fieldName, std::vector< T > fieldData, int dim0, int dim1, std::vector< int > perm)
- template<typename T >
  void writeMatlabField3 (mxArray ∗matlabStruct, const char ∗fieldName, std::vector< T > fieldData, int dim0, int dim1, int dim2, std::vector< int > perm)
- template<typename T >
  void writeMatlabField4 (mxArray ∗matlabStruct, const char ∗fieldName, std::vector< T > fieldData, int dim0, int dim1, int dim2, int dim3, std::vector< int > perm)
- double ∗ initAndAttachArray (mxArray ∗matlabStruct, const char ∗fieldName, std::vector< mwSize > dim)
- void checkFieldNames (const char ∗∗fieldNames, const int fieldCount)
- template<typename T >
  std::vector< T > reorder (const std::vector< T > input, const std::vector< int > order)
- template<typename T >
  char ∗ serializeToChar (T const &data, int ∗size)
- template<typename T >
  T deserializeFromChar (const char ∗buffer, int size)
- template<typename T >
  std::string serializeToString (T const &data)
- template<typename T >
  std::vector< char > serializeToStdVec (T const &data)

- template<typename T >
  T deserializeFromString (std::string const &serialized)
- bool operator== (const Solver &a, const Solver &b)
- int spline (int n, int end1, int end2, double slope1, double slope2, double x[ ], double y[ ], double b[ ], double c[ ], double d[ ])
- double seval (int n, double u, double x[ ], double y[ ], double b[ ], double c[ ], double d[ ])

  Evaluate the cubic spline function.
- double sinteg (int n, double u, double x[ ], double y[ ], double b[ ], double c[ ], double d[ ])
- double log (double x)
- double dirac (double x)
- double heaviside (double x)
- double min (double a, double b, double c)
- double Dmin (int id, double a, double b, double c)
- double max (double a, double b, double c)
- double Dmax (int id, double a, double b, double c)
- double pos_pow (double base, double exponent)
- int isNaN (double what)
- int isInf (double what)
- double getNaN ()
- double sign (double x)
- double spline (double t, int num,...)
- double spline_pos (double t, int num,...)
- double Dspline (int id, double t, int num,...)
- double Dspline_pos (int id, double t, int num,...)
- double DDspline (int id1, int id2, double t, int num,...)
- double DDspline_pos (int id1, int id2, double t, int num,...)
- def runAmiciSimulation (model, solver, edata=None)

  Convenience wrapper around amici.runAmiciSimulation (generated by swig)
- def ExpData (args)

  Convenience wrapper for ExpData constructors.
- def runAmiciSimulations (model, solver, edata_list, num_threads=1)

  Convenience wrapper for loops of amici.runAmiciSimulation.
- int dbl2int (const double x)
- char amici_blasCBlasTransToBlasTrans (BLASTranspose trans)
- std::vector< realtype > mxArrayToVector (const mxArray *array, int length)
- realtype getValueById (std::vector< std::string > const &ids, std::vector< realtype > const &values, std↩::string const &id, const char *variable_name, const char *id_name)

  local helper function to get parameters
- void setValueById (std::vector< std::string > const &ids, std::vector< realtype > &values, realtype value, std::string const &id, const char *variable_name, const char *id_name)

  local helper function to set parameters
- int setValueByIdRegex (std::vector< std::string > const &ids, std::vector< realtype > &values, realtype value, std::string const &regex, const char *variable_name, const char *id_name)

  local helper function to set parameters via regex

Variables

- msgIdAndTxtFp errMsgIdAndTxt = &printErrMsgIdAndTxt
- msgIdAndTxtFp warnMsgIdAndTxt = &printWarnMsgIdAndTxt
- constexpr double pi = 3.14159265358979323846
- bool hdf5_enabled = False

  boolean indicating if amici was compiled with hdf5 support
- bool has_clibs = False

boolean indicating if this is the full package with swig interface or the raw package without

- amici_path

  absolute root path of the amici repository

- amiciSwigPath = os.path.join(amici_path, 'swig')

  absolute path of the amici swig directory

- amiciSrcPath = os.path.join(amici_path, 'src')

  absolute path of the amici source directory

- amiciModulePath = os.path.dirname(__file__)

  absolute root path of the amici module

9.1.1 Detailed Description

The AMICI Python module provides functionality for importing SBML models and turning them into C++ Python extensions.

Getting started:

```
 creating a extension module for an SBML model:
import amici
amiSbml = amici.SbmlImporter('mymodel.sbml')
amiSbml.sbml2amici('modelName', 'outputDirectory')

 using the created module (set python path)
import modelName
help(modelName)
```

9.1.2 Typedef Documentation

9.1.2.1 realtype

```
typedef double realtype
```

defines variable type for simulation variables (determines numerical accuracy)

Definition at line 51 of file defines.h.

9.1.2.2 msgIdAndTxtFp

```
typedef void(* msgIdAndTxtFp) (const char *identifier, const char *format,...)
```

Parameters

identifier	string with error message identifier
format	string with error message printf-style format
...	arguments to be formatted

Definition at line 159 of file defines.h.

9.1.3 Enumeration Type Documentation

9.1.3.1 BLASLayout

`enum BLASLayout [strong]`

BLAS Matrix Layout, affects dgemm and gemv calls

Definition at line 54 of file defines.h.

9.1.3.2 BLASTranspose

`enum BLASTranspose [strong]`

BLAS Matrix Transposition, affects dgemm and gemv calls

Definition at line 60 of file defines.h.

9.1.3.3 ParameterScaling

`enum ParameterScaling [strong]`

modes for parameter transformations

Definition at line 67 of file defines.h.

9.1.3.4 SecondOrderMode

`enum SecondOrderMode [strong]`

modes for second order sensitivity analysis

Definition at line 74 of file defines.h.

9.1.3.5 SensitivityOrder

`enum SensitivityOrder [strong]`

orders of sensitivity analysis

Definition at line 81 of file defines.h.

9.1.3.6 SensitivityMethod

```
enum SensitivityMethod [strong]
```

methods for sensitivity computation

Definition at line 88 of file defines.h.

9.1.3.7 LinearSolver

```
enum LinearSolver [strong]
```

linear solvers for CVODES/IDAS

Definition at line 95 of file defines.h.

9.1.3.8 InternalSensitivityMethod

```
enum InternalSensitivityMethod [strong]
```

CVODES/IDAS forward sensitivity computation method

Definition at line 108 of file defines.h.

9.1.3.9 InterpolationType

```
enum InterpolationType [strong]
```

CVODES/IDAS state interpolation for adjoint sensitivity analysis

Definition at line 115 of file defines.h.

9.1.3.10 LinearMultistepMethod

```
enum LinearMultistepMethod [strong]
```

CVODES/IDAS linear multistep method

Definition at line 121 of file defines.h.

9.1.3.11 NonlinearSolverIteration

```
enum NonlinearSolverIteration [strong]
```

CVODES/IDAS Nonlinear Iteration method

Definition at line 127 of file defines.h.

9.1.3.12 StateOrdering

```
enum StateOrdering [strong]
```

KLU state reordering

Definition at line 133 of file defines.h.

9.1.3.13 SteadyStateSensitivityMode

```
enum SteadyStateSensitivityMode [strong]
```

Sensitivity computation mode in steadyStateProblem

Definition at line 140 of file defines.h.

9.1.3.14 NewtonStatus

```
enum NewtonStatus [strong]
```

State in which the steady state computionat finished

Definition at line 146 of file defines.h.

9.1.4 Function Documentation

9.1.4.1 printErrMsgIdAndTxt()

```
void printErrMsgIdAndTxt (
            const char * identifier,
            const char * format,
             ...  )
```

printErrMsgIdAndTxt prints a specified error message associated to the specified identifier

Parameters

in	*identifier*	error identifier **Type**: char
in	*format*	string with error message printf-style format
	...	arguments to be formatted

Returns

void

Definition at line 113 of file amici.cpp.

9.1.4.2 printWarnMsgIdAndTxt()

```
void printWarnMsgIdAndTxt (
            const char * identifier,
            const char * format,
             ...  )
```

printErrMsgIdAndTxt prints a specified warning message associated to the specified identifier

Parameters

in	*identifier*	warning identifier **Type**: char
in	*format*	string with error message printf-style format
	...	arguments to be formatted

Returns

void

Definition at line 134 of file amici.cpp.

9.1.4.3 runAmiciSimulation() [1/2]

```
std::unique_ptr< ReturnData > runAmiciSimulation (
            Solver & solver,
            const ExpData * edata,
            Model & model )
```

runAmiciSimulation is the core integration routine. It initializes the solver and runs the forward and backward problem.

Parameters

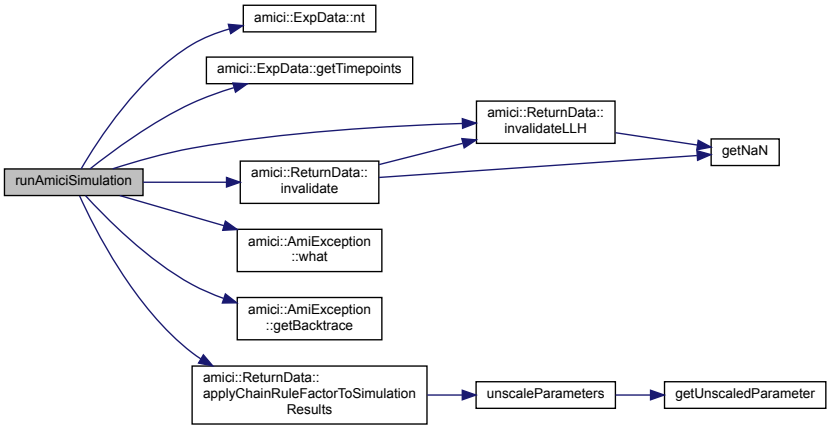
solver	Solver instance
edata	pointer to experimental data object
model	Model specification object

Returns

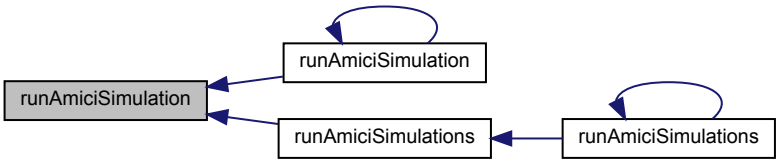
rdata pointer to return data object

Definition at line 42 of file amici.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.1.4.4 runAmiciSimulations() [1/2]

```
std::vector< std::unique_ptr< ReturnData > > runAmiciSimulations (
            Solver const & solver,
            const std::vector< ExpData *> & edatas,
            Model const & model,
            int num_threads )
```

runAmiciSimulations does the same as runAmiciSimulation, but for multiple ExpData instances.

Parameters

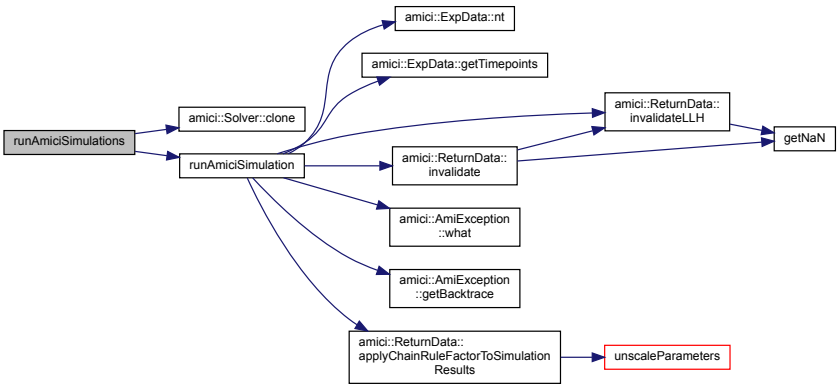
solver	Solver instance
edatas	experimental data objects
model	model specification object
num_threads	number of threads for parallel execution

Returns

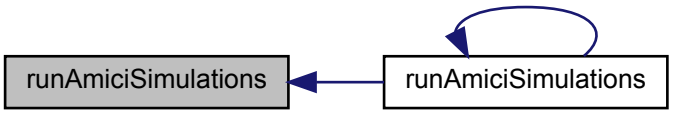
vector of pointers to return data objects

Definition at line 146 of file amici.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.1.4.5 amici_dgemv()

```
void amici_dgemv (
            BLASLayout layout,
            BLASTranspose TransA,
            const int M,
            const int N,
            const double alpha,
            const double * A,
            const int lda,
            const double * X,
            const int incX,
            const double beta,
            double * Y,
            const int incY )
```

amici_dgemm provides an interface to the blas matrix vector multiplication routine dgemv. This routines computes y = alpha∗A∗x + beta∗y with A: [MxK] B:[KxN] C:[MxN]

Parameters

in	*layout*	can be AMICI_BLAS_ColMajor or AMICI_BLAS_RowMajor.
in	*TransA*	flag indicating whether A should be transposed before multiplication
in	*M*	number of rows in A
in	*N*	number of columns in A
in	*alpha*	coefficient alpha
in	*A*	matrix A
in	*lda*	leading dimension of A (m or n)
in	*X*	vector X
in	*incX*	increment for entries of X
in	*beta*	coefficient beta
in,out	*Y*	vector Y
in	*incY*	increment for entries of Y

amici_dgemm provides an interface to the CBlas matrix vector multiplication routine dgemv. This routines computes y = alpha∗A∗x + beta∗y with A: [MxN] x:[Nx1] y:[Mx1]

Parameters

layout	always needs to be AMICI_BLAS_ColMajor.
TransA	flag indicating whether A should be transposed before multiplication
M	number of rows in A
N	number of columns in A
alpha	coefficient alpha
A	matrix A
lda	leading dimension of A (m or n)
X	vector X
incX	increment for entries of X
beta	coefficient beta
Y	vector Y
incY	increment for entries of Y

Returns

void

Definition at line 73 of file cblas.cpp.

9.1.4.6 amici_dgemm()

```
void amici_dgemm (
            BLASLayout layout,
            BLASTranspose TransA,
            BLASTranspose TransB,
            const int M,
            const int N,
            const int K,
            const double alpha,
```

```
const double * A,
const int lda,
const double * B,
const int ldb,
const double beta,
double * C,
const int ldc )
```

amici_dgemm provides an interface to the blas matrix matrix multiplication routine dgemm. This routines computes C = alpha∗A∗B + beta∗C with A: [MxK] B:[KxN] C:[MxN]

Parameters

in	*layout*	can be AMICI_BLAS_ColMajor or AMICI_BLAS_RowMajor.
in	*TransA*	flag indicating whether A should be transposed before multiplication
in	*TransB*	flag indicating whether B should be transposed before multiplication
in	*M*	number of rows in A/C
in	*N*	number of columns in B/C
in	*K*	number of rows in B, number of columns in A
in	*alpha*	coefficient alpha
in	*A*	matrix A
in	*lda*	leading dimension of A (m or k)
in	*B*	matrix B
in	*ldb*	leading dimension of B (k or n)
in	*beta*	coefficient beta
in,out	*C*	matrix C
in	*ldc*	leading dimension of C (m or n)

amici_dgemm provides an interface to the CBlas matrix matrix multiplication routine dgemm. This routines computes C = alpha∗A∗B + beta∗C with A: [MxK] B:[KxN] C:[MxN]

Parameters

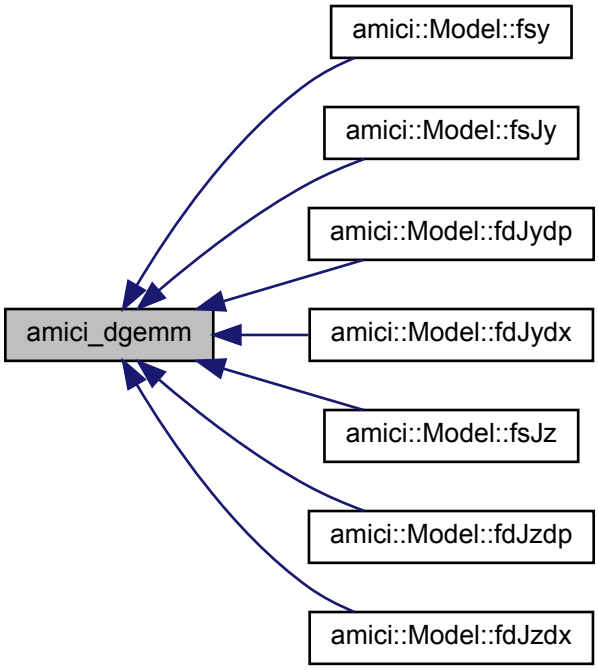
layout	memory layout.
TransA	flag indicating whether A should be transposed before multiplication
TransB	flag indicating whether B should be transposed before multiplication
M	number of rows in A/C
N	number of columns in B/C
K	number of rows in B, number of columns in A
alpha	coefficient alpha
A	matrix A
lda	leading dimension of A (m or k)
B	matrix B
ldb	leading dimension of B (k or n)
beta	coefficient beta
C	matrix C
ldc	leading dimension of C (m or n)

Returns

void

Definition at line 44 of file cblas.cpp.

Here is the caller graph for this function:



9.1.4.7 amici_daxpy()

```
void amici_daxpy (
            int n,
            double alpha,
            const double * x,
            const int incx,
            double * y,
            int incy )
```

Parameters

n	number of elements in y
alpha	scalar coefficient of x
x	vector of length n∗incx
incx	x stride
y	vector of length n∗incy
incy	y stride

Definition at line 90 of file cblas.cpp.

9.1.4.8 setModelData()

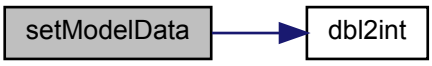
```
void setModelData (
            const mxArray * prhs[],
            int nrhs,
            Model & model )
```

Parameters

in	*prhs*	pointer to the array of input arguments **Type**: mxArray
in	*nrhs*	number of elements in prhs
in,out	*model*	model to update

Definition at line 389 of file interface_matlab.cpp.

Here is the call graph for this function:



9.1.4.9 setSolverOptions()

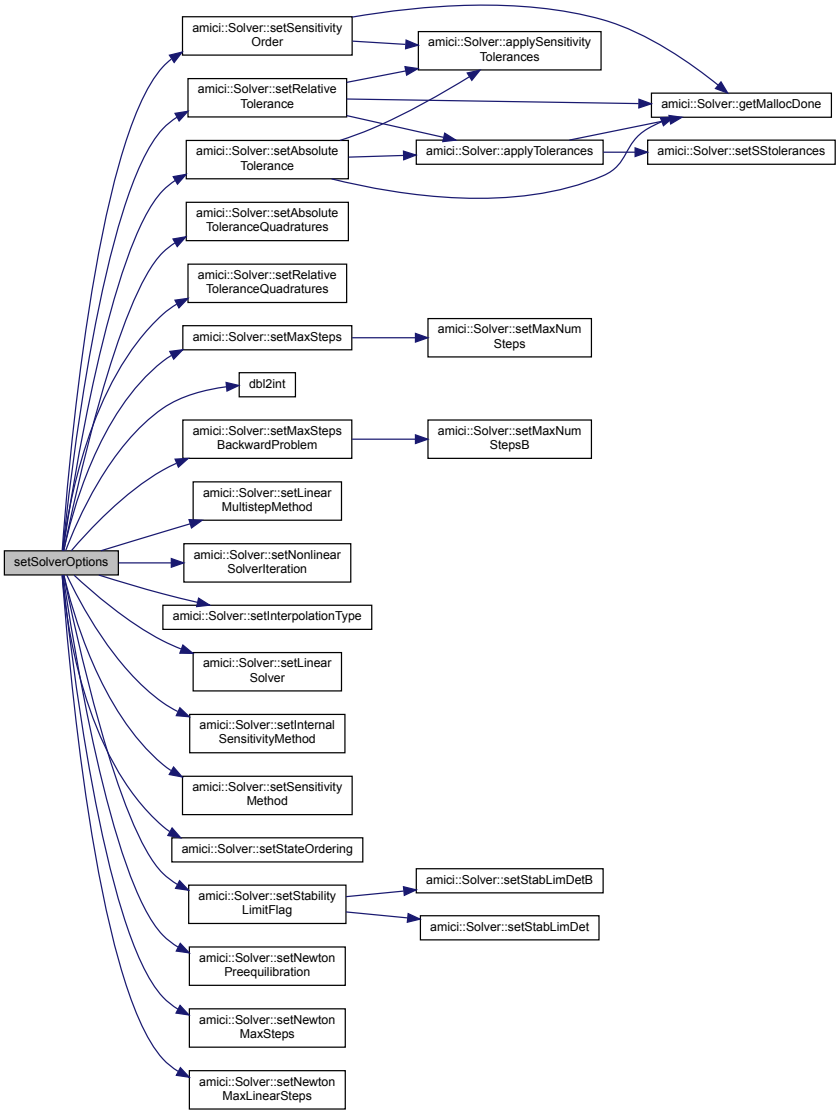
```
void setSolverOptions (
            const mxArray * prhs[],
            int nrhs,
            Solver & solver )
```

Parameters

in	*prhs*	pointer to the array of input arguments **Type**: mxArray
in	*nrhs*	number of elements in prhs
in,out	*solver*	solver to update

Definition at line 304 of file interface_matlab.cpp.

Here is the call graph for this function:



9.1.4.10 setupReturnData()

```
ReturnDataMatlab* amici::setupReturnData (
            mxArray * plhs[],
            int nlhs )
```

setupReturnData initialises the return data struct

Parameters

in	*plhs*	user input **Type**: mxArray
in	*nlhs*	number of elements in plhs **Type**: mxArray

Returns

rdata: return data struct
Type: ∗ReturnData

9.1.4.11 expDataFromMatlabCall()

```
std::unique_ptr< ExpData > expDataFromMatlabCall (
            const mxArray * prhs[],
            const Model & model )
```

expDataFromMatlabCall initialises the experimental data struct

Parameters

in	*prhs*	user input **Type**: ∗mxArray

Returns

edata: experimental data struct
Type: ∗ExpData

expDataFromMatlabCall parses the experimental data from the matlab call and writes it to an ExpData class object

Parameters

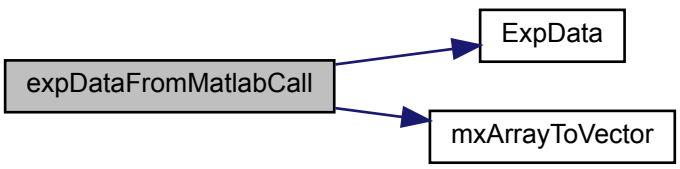
prhs	pointer to the array of input arguments
model	pointer to the model object, this is necessary to perform dimension checks

Returns

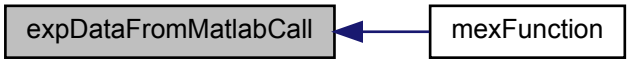
edata pointer to experimental data object

Definition at line 179 of file interface_matlab.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.1.4.12 checkFinite()

```
int checkFinite (
            const int N,
            const realtype * array,
            const char * fun )
```

Checks the values in an array for NaNs and Infs

Parameters

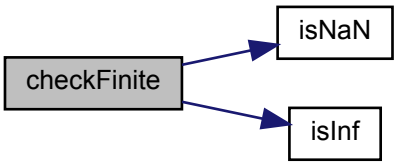
N	number of elements in array
array	array
fun	name of calling function

Returns

AMICI_RECOVERABLE_ERROR if a NaN/Inf value was found, AMICI_SUCCESS otherwise

Definition at line 17 of file misc.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

9.1.4.13 unscaleParameters() [1/2]

```
void unscaleParameters (
            const double * bufferScaled,
            const ParameterScaling * pscale,
            int n,
            double * bufferUnscaled )
```

Parameters

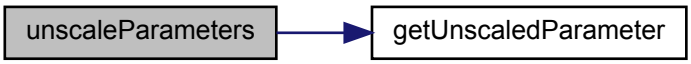
bufferScaled	scaled parameters
pscale	parameter scaling
n	number of elements in bufferScaled, pscale and bufferUnscaled
bufferUnscaled	unscaled parameters are written to the array

Returns

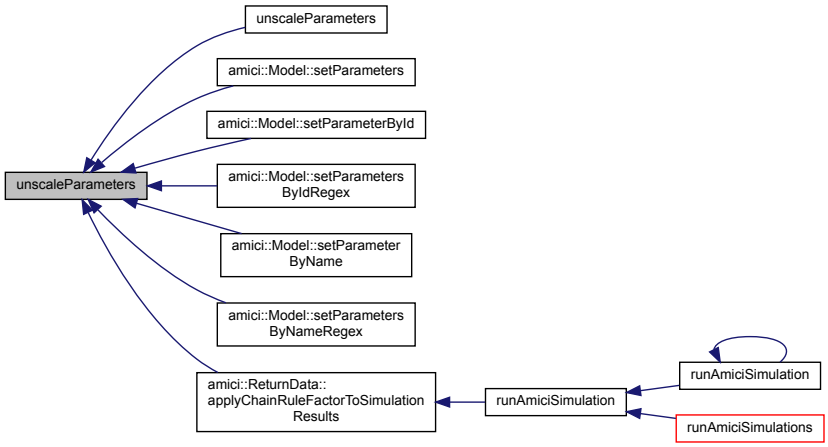
status flag indicating success of execution
Type: int

Definition at line 46 of file misc.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.1.4.14 unscaleParameters() [2/2]

```
void unscaleParameters (
            std::vector< double > const & bufferScaled,
            std::vector< ParameterScaling > const & pscale,
            std::vector< double > & bufferUnscaled )
```

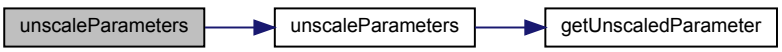
All vectors must be of same length

Parameters

bufferScaled	scaled parameters
pscale	parameter scaling
bufferUnscaled	unscaled parameters are written to the array

Definition at line 54 of file misc.cpp.

Here is the call graph for this function:



9.1.4.15 getUnscaledParameter()

```
double getUnscaledParameter (
            double scaledParameter,
            ParameterScaling scaling )
```

Parameters

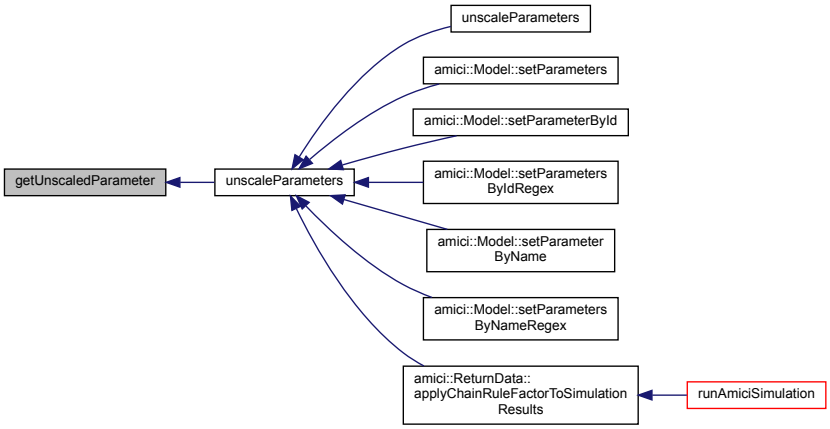
scaledParameter	scaled parameter
scaling	parameter scaling

Returns

Unscaled parameter

Definition at line 32 of file misc.cpp.

Here is the caller graph for this function:



9.1.4.16 getScaledParameter()

```
double getScaledParameter (
            double unscaledParameter,
            ParameterScaling scaling )
```

Parameters

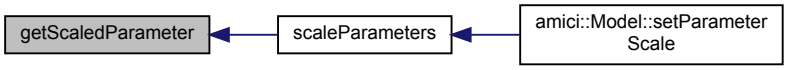
unscaledParameter	
scaling	parameter scaling

Returns

Scaled parameter

Definition at line 61 of file misc.cpp.

Here is the caller graph for this function:



9.1.4.17 scaleParameters()

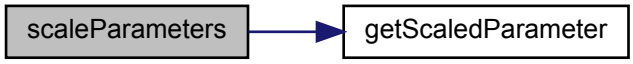
```
void scaleParameters (
            const std::vector< double > & bufferUnscaled,
            const std::vector< ParameterScaling > & pscale,
            std::vector< double > & bufferScaled )
```

Parameters

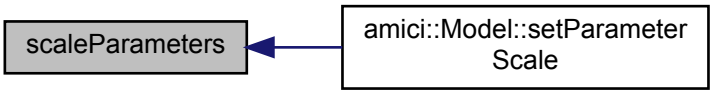
bufferUnscaled	
pscale	parameter scaling
bufferScaled	destination

Definition at line 76 of file misc.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.1.4.18 operator==() [1/2]

```
bool operator== (
            const Model & a,
            const Model & b )
```

Parameters

a	first model instance
b	second model instance

Returns

equality

Definition at line 1352 of file model.cpp.

9.1.4.19 getReturnDataMatlabFromAmiciCall()

```
mxArray * getReturnDataMatlabFromAmiciCall (
            ReturnData const * rdata )
```

generates matlab mxArray from a ReturnData object

Parameters

rdata	ReturnDataObject

Returns

rdatamatlab ReturnDataObject stored as matlab compatible data

generates matlab mxArray from a ReturnData object

Parameters

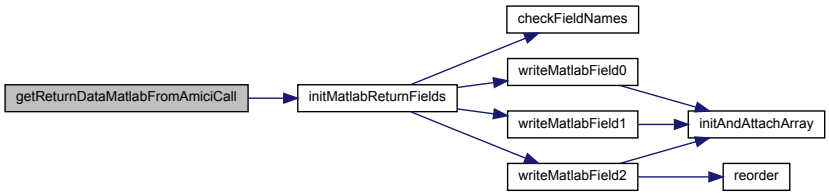
rdata	ReturnDataObject

Returns

rdatamatlab ReturnDataObject stored as matlab compatible data

Definition at line 7 of file returndata_matlab.cpp.

Here is the call graph for this function:



9.1.4.20 initMatlabReturnFields()

```
mxArray * initMatlabReturnFields (
            ReturnData const * rdata )
```

allocates and initialises solution mxArray with the corresponding fields

Parameters

rdata	ReturnDataObject

Returns

Solution mxArray

allocates and initialises solution mxArray with the corresponding fields

Parameters

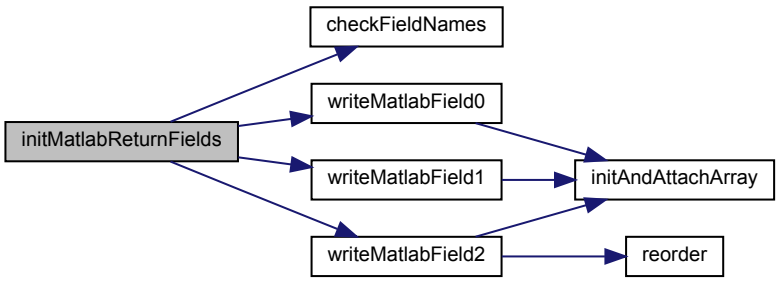
rdata	ReturnDataObject

Returns

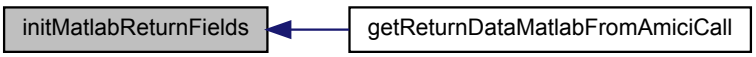
Solution mxArray

Definition at line 18 of file returndata_matlab.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.1.4.21 initMatlabDiagnosisFields()

```
mxArray * initMatlabDiagnosisFields (
            ReturnData const * rdata )
```

allocates and initialises diagnosis mxArray with the corresponding fields

Parameters

rdata	ReturnDataObject

Returns

Diagnosis mxArray

allocates and initialises diagnosis mxArray with the corresponding fields

Parameters

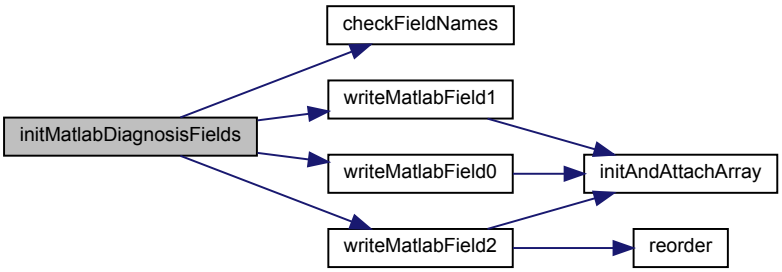
rdata	ReturnDataObject

Returns

Diagnosis mxArray

Definition at line 116 of file returndata_matlab.cpp.

Here is the call graph for this function:



9.1.4.22 writeMatlabField0()

```
void writeMatlabField0 (
            mxArray * matlabStruct,
            const char * fieldName,
            T fieldData )
```

initialise vector and attach to the field

Parameters

matlabStruct	pointer of the field to which the vector will be attached
fieldName	Name of the field to which the vector will be attached
fieldData	Data wich will be stored in the field

initialise vector and attach to the field

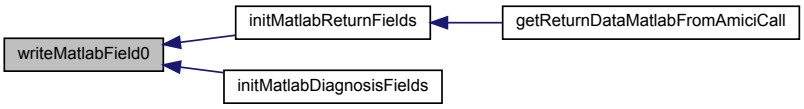
Parameters

matlabStruct	pointer of the field to which the vector will be attached
fieldName	Name of the field to which the vector will be attached
fieldData	Data wich will be stored in the field

Definition at line 181 of file returndata_matlab.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



9.1.4.23 writeMatlabField1()

```
void writeMatlabField1 (
            mxArray * matlabStruct,
            const char * fieldName,
            std::vector< T > fieldData,
            const int dim0 )
```

initialise vector and attach to the field

Parameters

matlabStruct	pointer of the field to which the vector will be attached
fieldName	Name of the field to which the vector will be attached
fieldData	Data wich will be stored in the field
dim0	Number of elements in the vector

initialise vector and attach to the field

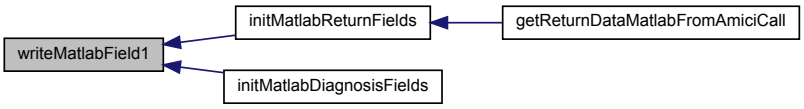
Parameters

matlabStruct	pointer of the field to which the vector will be attached
fieldName	Name of the field to which the vector will be attached
fieldData	Data wich will be stored in the field
dim0	Number of elements in the vector

Definition at line 199 of file returndata_matlab.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



9.1.4.24 writeMatlabField2()

```
void writeMatlabField2 (
            mxArray * matlabStruct,
            const char * fieldName,
            std::vector< T > fieldData,
            int dim0,
            int dim1,
            std::vector< int > perm )
```

initialise matrix, attach to the field and write data

Parameters

matlabStruct	Pointer to the matlab structure
fieldName	Name of the field to which the tensor will be attached
fieldData	Data wich will be stored in the field
dim0	Number of rows in the tensor
dim1	Number of columns in the tensor
perm	reordering of dimensions (i.e., transposition)

initialise matrix, attach to the field and write data

Parameters

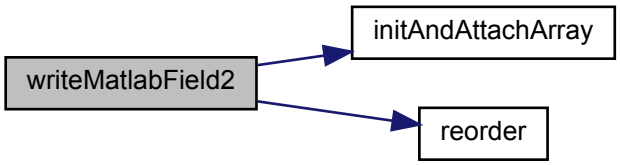
matlabStruct	Pointer to the matlab structure
fieldName	Name of the field to which the tensor will be attached
fieldData	Data wich will be stored in the field

Parameters

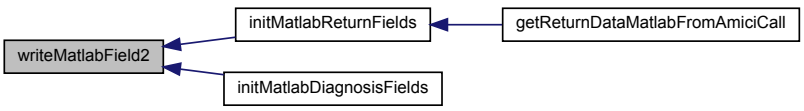
dim0	Number of rows in the tensor
dim1	Number of columns in the tensor
perm	reordering of dimensions (i.e., transposition)

Definition at line 221 of file returndata_matlab.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.1.4.25 writeMatlabField3()

```
void writeMatlabField3 (
            mxArray * matlabStruct,
            const char * fieldName,
            std::vector< T > fieldData,
            int dim0,
            int dim1,
            int dim2,
            std::vector< int > perm )
```

initialise 3D tensor, attach to the field and write data

Parameters

matlabStruct	Pointer to the matlab structure
fieldName	Name of the field to which the tensor will be attached
fieldData	Data wich will be stored in the field
dim0	number of rows in the tensor
dim1	number of columns in the tensor
dim2	number of elements in the third dimension of the tensor
perm	reordering of dimensions

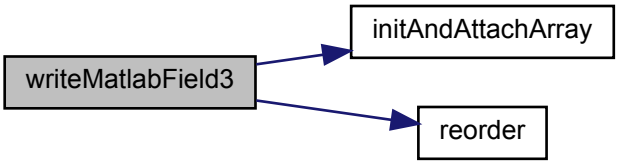
initialise 3D tensor, attach to the field and write data

Parameters

matlabStruct	Pointer to the matlab structure
fieldName	Name of the field to which the tensor will be attached
fieldData	Data wich will be stored in the field
dim0	number of rows in the tensor
dim1	number of columns in the tensor
dim2	number of elements in the third dimension of the tensor
perm	reordering of dimensions

Definition at line 254 of file returndata_matlab.cpp.

Here is the call graph for this function:



9.1.4.26 writeMatlabField4()

```
void writeMatlabField4 (
            mxArray * matlabStruct,
            const char * fieldName,
            std::vector< T > fieldData,
            int dim0,
            int dim1,
            int dim2,
            int dim3,
            std::vector< int > perm )
```

initialise 4D tensor, attach to the field and write data

Parameters

matlabStruct	Pointer to the matlab structure
fieldName	Name of the field to which the tensor will be attached
fieldData	Data wich will be stored in the field
dim0	number of rows in the tensor
dim1	number of columns in the tensor
dim2	number of elements in the third dimension of the tensor
dim3	number of elements in the fourth dimension of the tensor
perm	reordering of dimensions

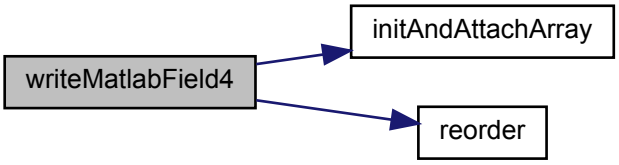
initialise 4D tensor, attach to the field and write data

Parameters

matlabStruct	Pointer to the matlab structure
fieldName	Name of the field to which the tensor will be attached
fieldData	Data wich will be stored in the field
dim0	number of rows in the tensor
dim1	number of columns in the tensor
dim2	number of elements in the third dimension of the tensor
dim3	number of elements in the fourth dimension of the tensor
perm	reordering of dimensions

Definition at line 290 of file returndata_matlab.cpp.

Here is the call graph for this function:



9.1.4.27 initAndAttachArray()

```
double * initAndAttachArray (
            mxArray * matlabStruct,
            const char * fieldName,
            std::vector< mwSize > dim )
```

initialises the field fieldName in matlabStruct with dimension dim

Parameters

matlabStruct	Pointer to the matlab structure
fieldName	Name of the field to which the tensor will be attached
dim	vector of field dimensions

Returns

Pointer to field data

initialises the field fieldName in matlabStruct with dimension dim

Parameters

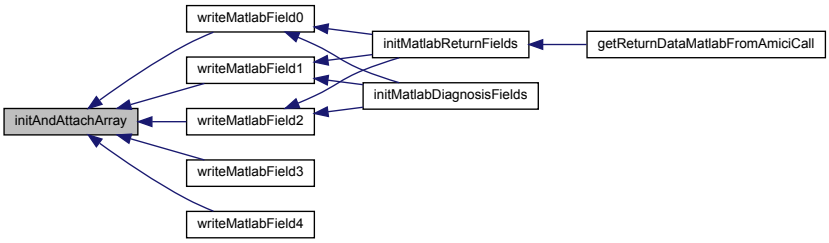
matlabStruct	Pointer to the matlab structure
fieldName	Name of the field to which the tensor will be attached
dim	vector of field dimensions

Returns

Pointer to field data

Definition at line 328 of file returndata_matlab.cpp.

Here is the caller graph for this function:



9.1.4.28 checkFieldNames()

```
void checkFieldNames (
            const char ** fieldNames,
            const int fieldCount )
```

checks whether fieldNames was properly allocated

Parameters

fieldNames	array of field names
fieldCount	expected number of fields in fieldNames

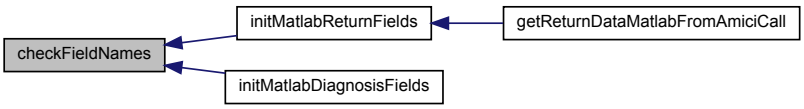
checks whether fieldNames was properly allocated

Parameters

fieldNames	array of field names
fieldCount	expected number of fields in fieldNames

Definition at line 349 of file returndata_matlab.cpp.

Here is the caller graph for this function:



9.1.4.29 reorder()

```
std::vector< T > reorder (
            const std::vector< T > input,
            const std::vector< int > order )
```

template function that reorders elements in a std::vector

Parameters

input	unordered vector
order	dimension permutation

Returns

Reordered vector

template function that reorders elements in a std::vector

Parameters

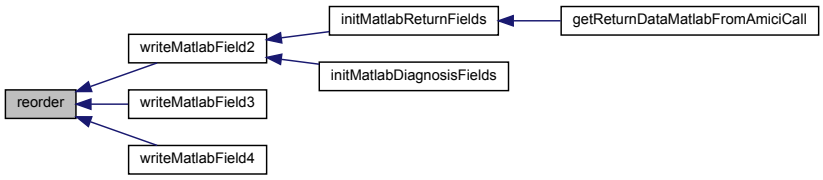
input	unordered vector
order	dimension permutation

Returns

Reordered vector

Definition at line 362 of file returndata_matlab.cpp.

Here is the caller graph for this function:



9.1.4.30 serializeToChar()

```
char* amici::serializeToChar (
            T const & data,
            int * size )
```

Serialize object to char array

Parameters

data	input object
size	maximum char length

Returns

The object serialized as char

Definition at line 177 of file serialization.h.

9.1.4.31 deserializeFromChar()

```
T amici::deserializeFromChar (
            const char * buffer,
            int size )
```

Deserialize object that has been serialized using serializeToChar

Parameters

buffer	serialized object
size	length of buffer

Returns

The deserialized object

Definition at line 210 of file serialization.h.

9.1.4.32 serializeToString()

```
std::string amici::serializeToString (
            T const & data )
```

Serialize object to string

Parameters

data	input object

Returns

The object serialized as string

Definition at line 235 of file serialization.h.

9.1.4.33 serializeToStdVec()

```
std::vector<char> amici::serializeToStdVec (
            T const & data )
```

Serialize object to std::vector<char>

Parameters

data	input object

Returns

The object serialized as std::vector<char>

Definition at line 261 of file serialization.h.

9.1.4.34 deserializeFromString()

```
T amici::deserializeFromString (
            std::string const & serialized )
```

Deserialize object that has been serialized using serializeToString

Parameters

serialized	serialized object

Returns

The deserialized object

Definition at line 288 of file serialization.h.

9.1.4.35 operator==() [2/2]

```
bool operator== (
            const Solver & a,
            const Solver & b )
```

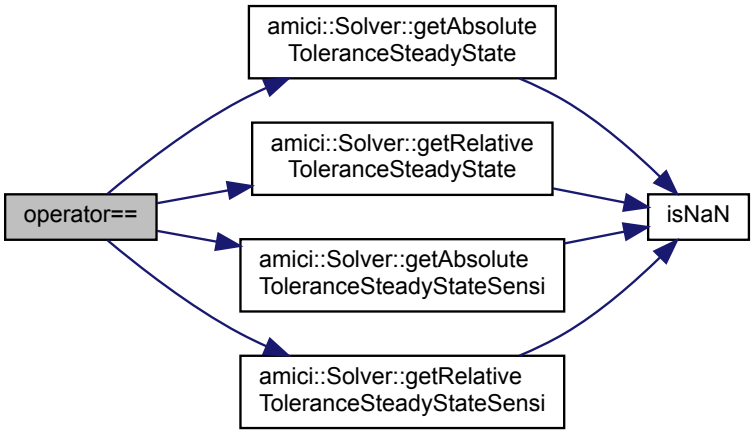
Parameters

a	
b	

Returns

Definition at line 378 of file solver.cpp.

Here is the call graph for this function:



9.1.4.36 spline() [1/2]

```
int spline (
            int n,
            int end1,
            int end2,
            double slope1,
            double slope2,
            double x[],
            double y[],
            double b[],
            double c[],
            double d[] )
```

Evaluate the coefficients b[i], c[i], d[i], i = 0, 1, .. n-1 for a cubic interpolating spline

S(xx) = Y[i] + b[i] ∗ w + c[i] ∗ w∗∗2 + d[i] ∗ w∗∗3 where w = xx - x[i] and x[i] <= xx <= x[i+1]

The n supplied data points are x[i], y[i], i = 0 ... n-1.

Parameters

in	*n*	The number of data points or knots (n >= 2)
in	*end1*	0: default condition 1: specify the slopes at x[0]
in	*end2*	0: default condition 1: specify the slopes at x[n-1]
in	*slope1*	slope at x[0]
in	*slope2*	slope at x[n-1]
in	*x[]*	the abscissas of the knots in strictly increasing order
in	*y[]*	the ordinates of the knots
out	*b[]*	array of spline coefficients
out	*c[]*	array of spline coefficients
out	*d[]*	array of spline coefficients

Return values

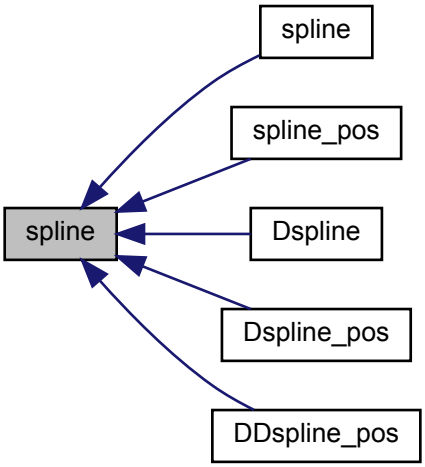
0	normal return
1	less than two data points; cannot interpolate
2	x[] are not in ascending order

Notes

- The accompanying function seval() may be used to evaluate the spline while deriv will provide the first derivative.
- Using p to denote differentiation y[i] = S(X[i]) b[i] = Sp(X[i]) c[i] = Spp(X[i])/2 d[i] = Sppp(X[i])/6 (Derivative from the right)
- Since the zero elements of the arrays ARE NOW used here, all arrays to be passed from the main program should be dimensioned at least [n]. These routines will use elements [0 .. n-1].
- Adapted from the text Forsythe, G.E., Malcolm, M.A. and Moler, C.B. (1977) "Computer Methods for Mathematical Computations" Prentice Hall
- Note that although there are only n-1 polynomial segments, n elements are requird in b, c, d. The elements b[n-1], c[n-1] and d[n-1] are set to continue the last segment past x[n-1].

Definition at line 16 of file spline.cpp.

Here is the caller graph for this function:



9.1.4.37 seval()

```
double seval (
            int n,
            double u,
            double x[],
            double y[],
            double b[],
            double c[],
            double d[] )
```

S(xx) = y[i] + b[i] ∗ w + c[i] ∗ w∗∗2 + d[i] ∗ w∗∗3 where w = u - x[i] and x[i] <= u <= x[i+1] Note that Horner's rule is used. If u < x[0] then i = 0 is used. If u > x[n-1] then i = n-1 is used.

Parameters

in	*n*	The number of data points or knots (n >= 2)
in	*u*	the abscissa at which the spline is to be evaluated
in	*x[]*	the abscissas of the knots in strictly increasing order
in	*y[]*	the ordinates of the knots
in	*b*	array of spline coefficients computed by spline().
in	*c*	array of spline coefficients computed by spline().
in	*d*	array of spline coefficients computed by spline().

Returns

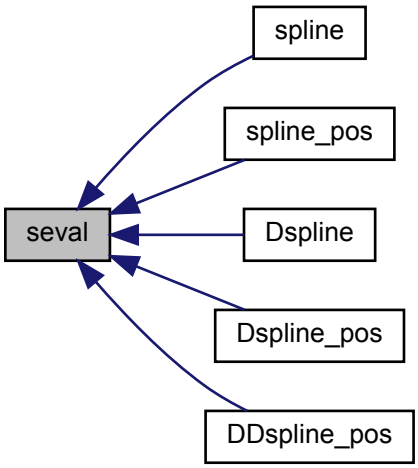
the value of the spline function at u

Notes

- If u is not in the same interval as the previous call then a binary search is performed to determine the proper interval.

Definition at line 195 of file spline.cpp.

Here is the caller graph for this function:



9.1.4.38 sinteg()

```
double sinteg (
            int n,
            double u,
            double x[],
            double y[],
            double b[],
            double c[],
            double d[] )
```

Integrate the cubic spline function

S(xx) = y[i] + b[i] ∗ w + c[i] ∗ w∗∗2 + d[i] ∗ w∗∗3 where w = u - x[i] and x[i] <= u <= x[i+1]

The integral is zero at u = x[0].

If u < x[0] then i = 0 segment is extrapolated. If u > x[n-1] then i = n-1 segment is extrapolated.

Parameters

in	*n*	the number of data points or knots (n >= 2)
in	*u*	the abscissa at which the spline is to be evaluated
in	*x[]*	the abscissas of the knots in strictly increasing order
in	*y[]*	the ordinates of the knots
in	*b*	array of spline coefficients computed by spline().
in	*c*	array of spline coefficients computed by spline().
in	*d*	array of spline coefficients computed by spline().

Returns

the value of the spline function at u

Notes

- If u is not in the same interval as the previous call then a binary search is performed to determine the proper interval.

Definition at line 256 of file spline.cpp.

9.1.4.39 log()

```
double log (
            double x )
```

c implementation of log function, this prevents returning NaN values for negative values

Parameters

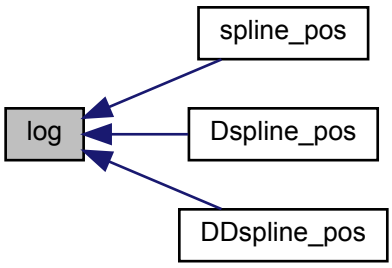
x	argument

Returns

if(x>0) then log(x) else -Inf

Definition at line 62 of file symbolic_functions.cpp.

Here is the caller graph for this function:



9.1.4.40 dirac()

```
double dirac (
            double x )
```

c implementation of matlab function dirac

Parameters

x	argument

Returns

if(x==0) then INF else 0

Definition at line 77 of file symbolic_functions.cpp.

9.1.4.41 heaviside()

```
double heaviside (
            double x )
```

c implementation of matlab function heaviside

Parameters

x	argument

Returns

if(x>0) then 1 else 0

Definition at line 92 of file symbolic_functions.cpp.

9.1.4.42 min()

```
double min (
            double a,
            double b,
            double c )
```

c implementation of matlab function min

Parameters

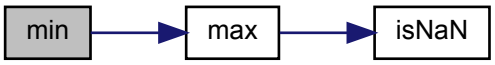
a	value1
b	value2
c	bogus parameter to ensure correct parsing as a function

Returns

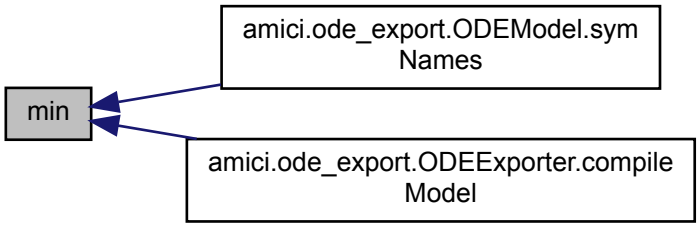
if(a < b) then a else b

Definition at line 149 of file symbolic_functions.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.1.4.43 Dmin()

```
double Dmin (
            int id,
            double a,
            double b,
            double c )
```

parameter derivative of c implementation of matlab function max

Parameters

id	argument index for differentiation
a	value1
b	value2
c	bogus parameter to ensure correct parsing as a function

Returns

id == 1: if(a > b) then 1 else 0
id == 2: if(a > b) then 0 else 1

Definition at line 191 of file symbolic_functions.cpp.

Here is the call graph for this function:

9.1.4.44 max()

```
double max (
            double a,
            double b,
            double c )
```

c implementation of matlab function max

Parameters

a	value1
b	value2
c	bogus parameter to ensure correct parsing as a function

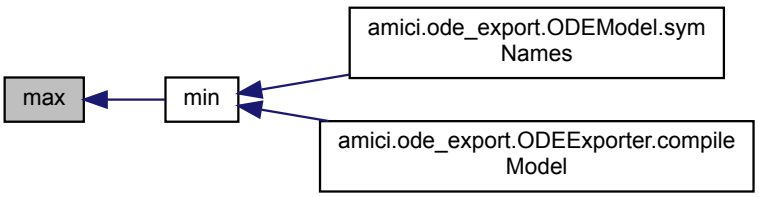
Returns

if(a > b) then a else b

Definition at line 128 of file symbolic_functions.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



9.1.4.45 Dmax()

```
double Dmax (
            int id,
            double a,
            double b,
            double c )
```

parameter derivative of c implementation of matlab function max

Parameters

id	argument index for differentiation
a	value1
b	value2
c	bogus parameter to ensure correct parsing as a function

Returns

id == 1: if(a > b) then 1 else 0
id == 2: if(a > b) then 0 else 1

Definition at line 164 of file symbolic_functions.cpp.

Here is the caller graph for this function:

9.1.4.46 pos_pow()

```
double pos_pow (
            double base,
            double exponent )
```

specialized pow functions that assumes positivity of the first argument

Parameters

base	base
exponent	exponent

Returns

pow(max(base,0.0),exponen)

Definition at line 203 of file symbolic_functions.cpp.

9.1.4.47 isNaN()

```
int isNaN (
            double what )
```

c++ interface to the isNaN function

Parameters

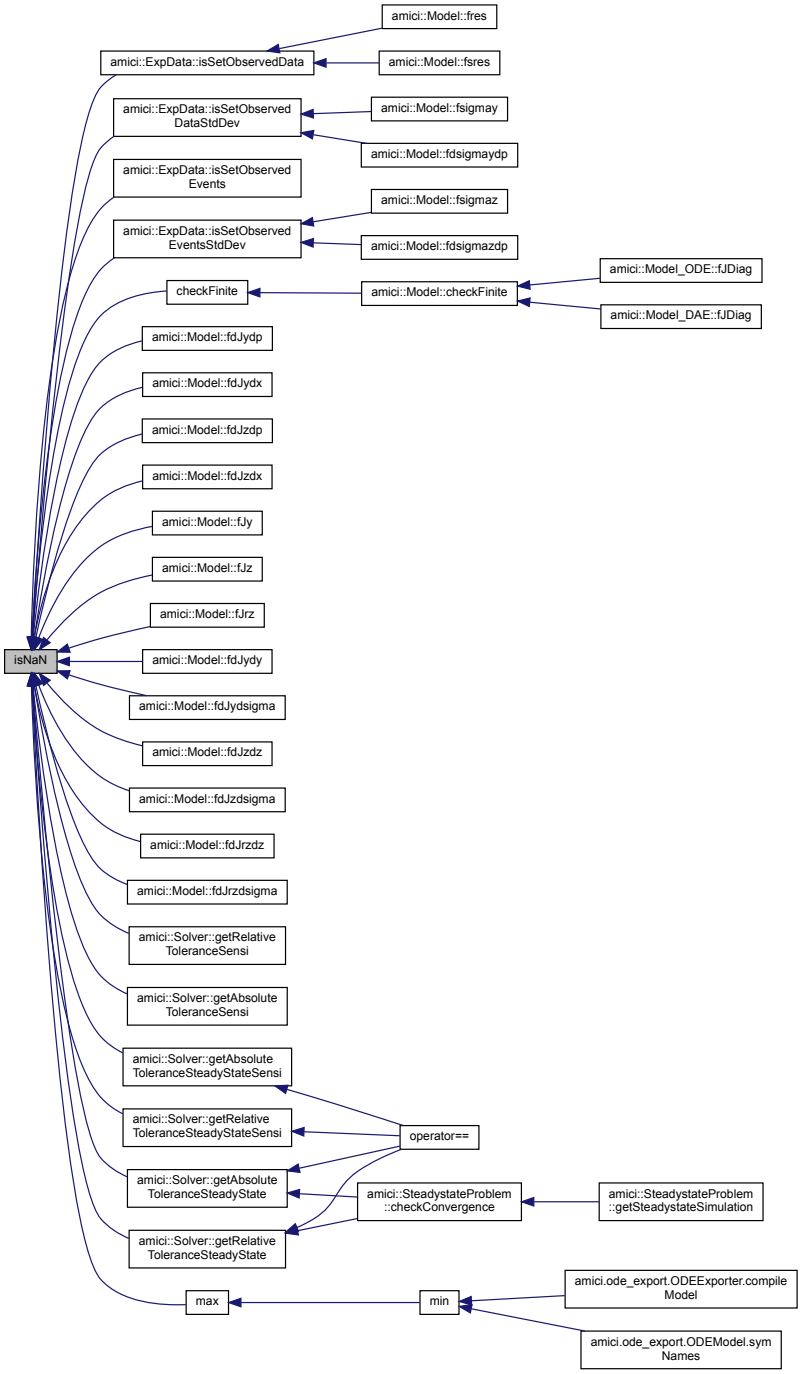
what	argument

Returns

isnan(what)

Definition at line 35 of file symbolic_functions.cpp.

Here is the caller graph for this function:



9.1.4.48 isInf()

```
int isInf (
            double what )
```

c++ interface to the isinf function

Parameters

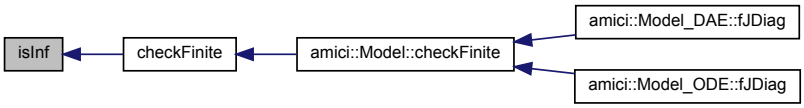
what	argument

Returns

isnan(what)

Definition at line 44 of file symbolic_functions.cpp.

Here is the caller graph for this function:



9.1.4.49 getNaN()

```
double getNaN ( )
```

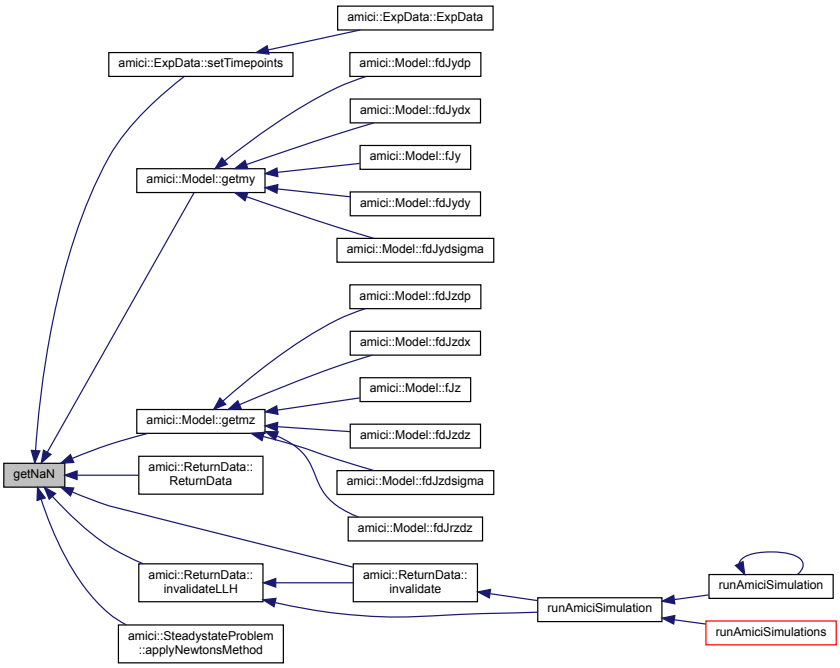
function returning nan

Returns

NaN

Definition at line 52 of file symbolic_functions.cpp.

Here is the caller graph for this function:



9.1.4.50 sign()

```
double sign (
            double x )
```

c implementation of matlab function sign

Parameters

x	argument

Returns

0

Definition at line 107 of file symbolic_functions.cpp.

9.1.4.51 spline() [2/2]

```
double spline (
            double t,
            int num,
             ...  )
```

spline function, takes variable argument pairs (ti,pi) with `ti`: location of node i and `pi`: spline value at node i. the last two arguments are always `ss`: flag indicating whether slope at first node should be user defined and `dudt` user defined slope at first node. All arguments must be of type double.

Parameters

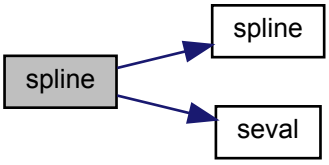
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

spline(t)

Definition at line 222 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.1.4.52 spline_pos()

```
double spline_pos (
            double t,
            int num,
             ...  )
```

exponentiated spline function, takes variable argument pairs (ti,pi) with `ti`: location of node i and `pi`: spline value at node i. the last two arguments are always `ss`: flag indicating whether slope at first node should be user defined and `dudt` user defined slope at first node. All arguments must be of type double.

Parameters

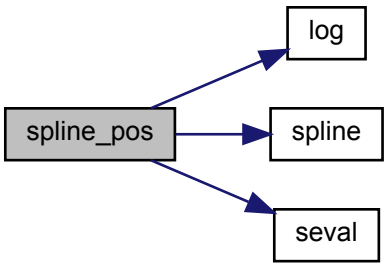
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

spline(t)

Definition at line 273 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.1.4.53 Dspline()

```
double Dspline (
            int id,
            double t,
            int num,
             ...  )
```

derivation of a spline function, takes variable argument pairs (ti,pi) with `ti`: location of node i and `pi`: spline value at node i. the last two arguments are always `ss`: flag indicating whether slope at first node should be user defined and `dudt` user defined slope at first node. All arguments but id must be of type double.

Parameters

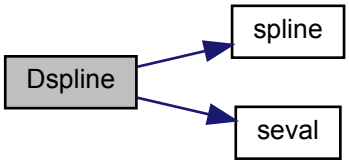
id	index of node to which the derivative of the corresponding spline coefficient should be computed
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

dsplinedp(t)

Definition at line 326 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.1.4.54 Dspline_pos()

```
double Dspline_pos (
            int id,
            double t,
            int num,
             ...  )
```

derivation of an exponentiated spline function, takes variable argument pairs (ti,pi) with `ti`: location of node i and `pi`: spline value at node i. the last two arguments are always `ss`: flag indicating whether slope at first node should be user defined and `dudt` user defined slope at first node. All arguments but id must be of type double.

Parameters

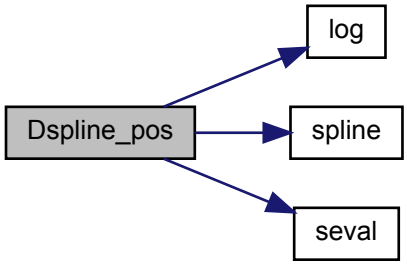
id	index of node to which the derivative of the corresponding spline coefficient should be computed
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

dsplinedp(t)

Definition at line 382 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.1.4.55 DDspline()

```
double DDspline (
            int id1,
            int id2,
            double t,
            int num,
             ...  )
```

second derivation of a spline function, takes variable argument pairs (ti,pi) with `ti`: location of node i and `pi`: spline value at node i. the last two arguments are always `ss`: flag indicating whether slope at first node should be user defined and `dudt` user defined slope at first node. All arguments but id1 and id2 must be of type double.

Parameters

id1	index of node to which the first derivative of the corresponding spline coefficient should be computed
id2	index of node to which the second derivative of the corresponding spline coefficient should be computed
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

ddspline(t)

Definition at line 448 of file symbolic_functions.cpp.

9.1.4.56 DDspline_pos()

```
double DDspline_pos (
            int id1,
```

```
int id2,
double t,
int num,
 ...  )
```

derivation of an exponentiated spline function, takes variable argument pairs (ti,pi) with `ti`: location of node i and `pi`: spline value at node i. the last two arguments are always `ss`: flag indicating whether slope at first node should be user defined and `dudt` user defined slope at first node. All arguments but id1 and id2 must be of type double.

Parameters

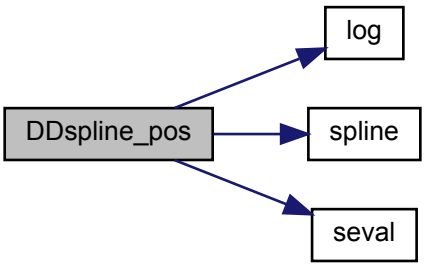
id1	index of node to which the first derivative of the corresponding spline coefficient should be computed
id2	index of node to which the second derivative of the corresponding spline coefficient should be computed
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

ddspline(t)

Definition at line 468 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.1.4.57 runAmiciSimulation() [2/2]

```
def amici.runAmiciSimulation (
              model,
              solver,
              edata = None )
```

Parameters

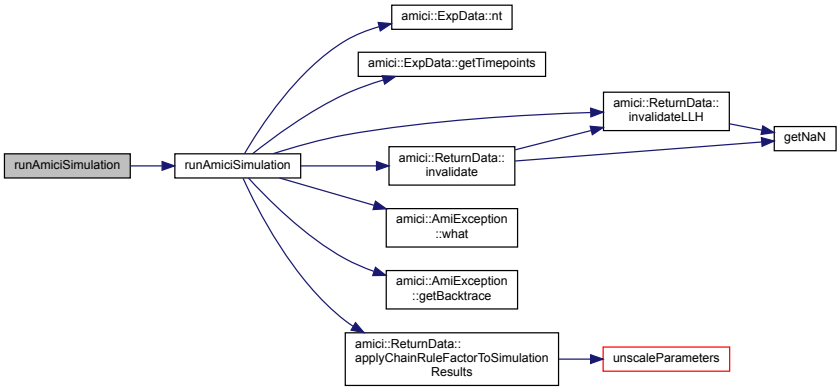
model	Model instance
solver	Solver instance, must be generated from Model.getSolver()
edata	ExpData instance (optional)

Returns

ReturnData object with simulation results

Definition at line 93 of file __init__.py.

Here is the call graph for this function:



Here is the caller graph for this function:

9.1.4.58 ExpData()

```
def amici.ExpData (
            args )
```

Parameters

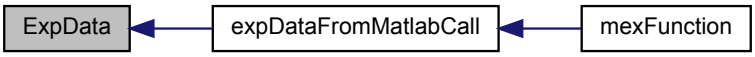
args	arguments

Returns

ExpData Instance

Definition at line 112 of file __init__.py.

Here is the caller graph for this function:



9.1.4.59 runAmiciSimulations() [2/2]

```
def amici.runAmiciSimulations (
              model,
              solver,
              edata_list,
              num_threads = 1 )
```

Parameters

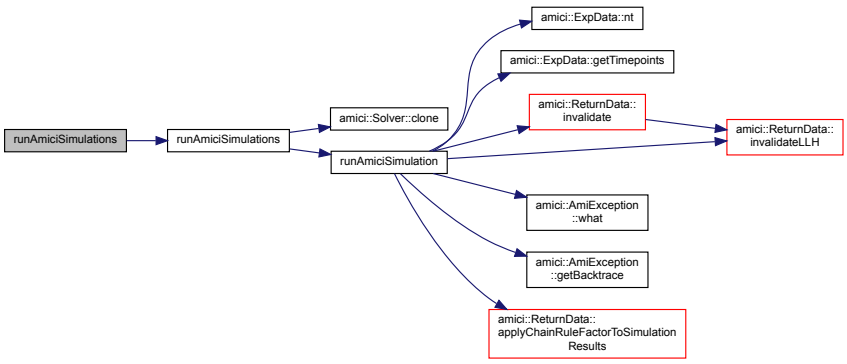
model	Model instance
solver	Solver instance, must be generated from Model.getSolver()
edata_list	list of ExpData instances
num_threads	number of threads to use (only used if compiled with openmp)

Returns

list of ReturnData objects with simulation results

Definition at line 140 of file __init__.py.

Here is the call graph for this function:



Here is the caller graph for this function:

9.1.4.60 dbl2int()

```
int dbl2int (
            const double x )
```

conversion from double to int with checking for loss of data

Parameters

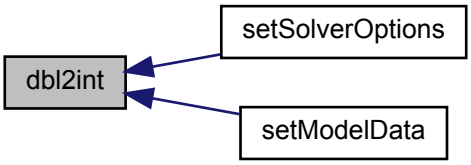
x	input

Returns

int_x casted value

Definition at line 298 of file interface_matlab.cpp.

Here is the caller graph for this function:



9.1.4.61 amici_blasCBlasTransToBlasTrans()

```
char amici::amici_blasCBlasTransToBlasTrans (
            BLASTranspose trans )
```

amici_blasCBlasTransToBlasTrans translates AMICI_BLAS_TRANSPOSE values to CBlas readable strings

Parameters

trans	flag indicating transposition and complex conjugation

Returns

cblastrans CBlas readable CHAR indicating transposition and complex conjugation

Definition at line 52 of file interface_matlab.cpp.

9.1.4.62 mxArrayToVector()

```
std::vector<realtype> amici::mxArrayToVector (
            const mxArray * array,
            int length )
```

conversion from mxArray to vector<realtype>

Parameters

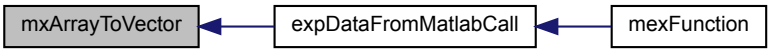
array	Matlab array to create vector from
length	Number of elements in array

Returns

std::vector with data from array

Definition at line 166 of file interface_matlab.cpp.

Here is the caller graph for this function:



9.1.4.63 getValueById()

```
realtype amici::getValueById (
            std::vector< std::string > const & ids,
            std::vector< realtype > const & values,
            std::string const & id,
            const char * variable_name,
            const char * id_name )
```

Parameters

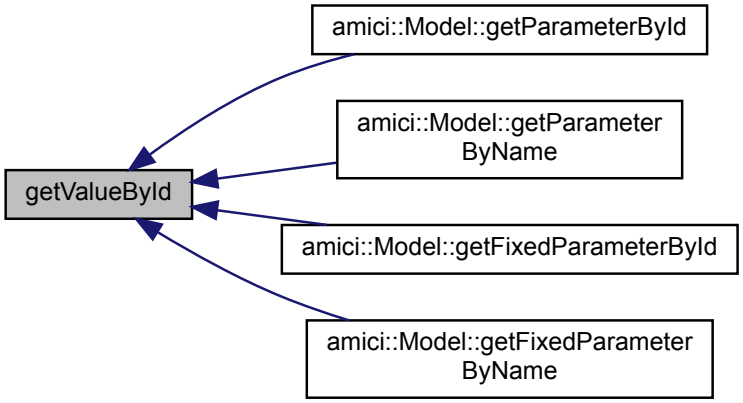
ids	vector of name/ids of (fixed)Parameters
values	values of the (fixed)Parameters
id	name/id to look for in the vector
variable_name	string indicating what variable we are lookin at
id_name	string indicating whether name or id was specified

Returns

value of the selected parameter

Definition at line 319 of file model.cpp.

Here is the caller graph for this function:



9.1.4.64 setValueById()

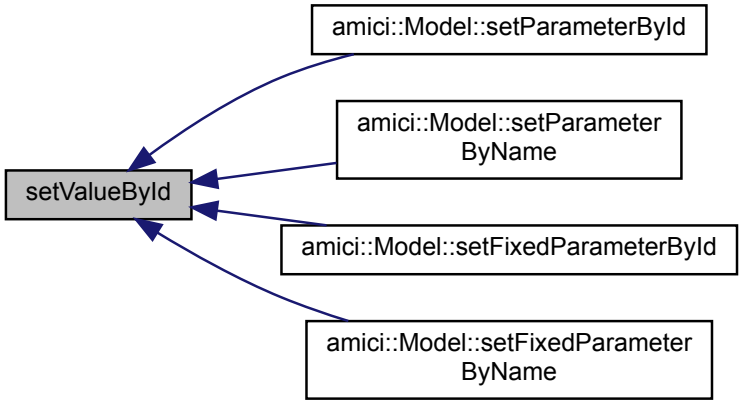
```
void amici::setValueById (
            std::vector< std::string > const & ids,
            std::vector< realtype > & values,
            realtype value,
            std::string const & id,
            const char * variable_name,
            const char * id_name )
```

Parameters

ids	vector of names/ids of (fixed)Parameters
values	values of the (fixed)Parameters
value	for the selected parameter
id	name/id to look for in the vector
variable_name	string indicating what variable we are lookin at
id_name	string indicating whether name or id was specified

Definition at line 337 of file model.cpp.

Here is the caller graph for this function:



9.1.4.65 setValueByIdRegex()

```
int amici::setValueByIdRegex (
            std::vector< std::string > const & ids,
            std::vector< realtype > & values,
            realtype value,
            std::string const & regex,
            const char * variable_name,
            const char * id_name )
```

Parameters

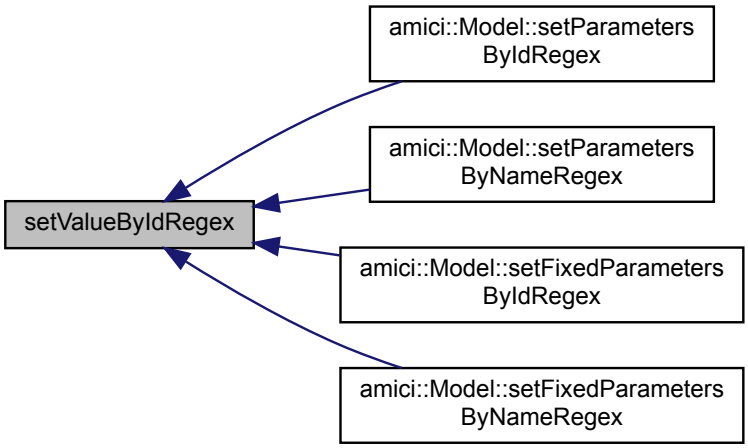
ids	vector of names/ids of (fixed)Parameters
values	values of the (fixed)Parameters
value	for the selected parameter
regex	string according to which names/ids are to be matched
variable_name	string indicating what variable we are lookin at
id_name	string indicating whether name or id was specified

Returns

number of matched names/ids

Definition at line 356 of file model.cpp.

Here is the caller graph for this function:



9.1.5 Variable Documentation

9.1.5.1 errMsgIdAndTxt

```
msgIdAndTxtFp errMsgIdAndTxt = &printErrMsgIdAndTxt
```

errMsgIdAndTxt is a function pointer for printErrMsgIdAndTxt

Definition at line 37 of file amici.cpp.

9.1.5.2 warnMsgIdAndTxt

```
msgIdAndTxtFp warnMsgIdAndTxt = &printWarnMsgIdAndTxt
```

warnMsgIdAndTxt is a function pointer for printWarnMsgIdAndTxt

Definition at line 13 of file model_dae.h.

9.1.5.3 pi

```
constexpr double pi = 3.14159265358979323846
```

MS definition of PI and other constants

Definition at line 13 of file defines.h.

9.1.5.4 amici_path

`amici_path`

Initial value:

```
1 =  os.path.abspath(os.path.join(
2         os.path.dirname(__file__), '..', '..'))
```

Definition at line 55 of file __init__.py.

9.2 amici.ode_export Namespace Reference

The C++ ODE export module for python.

Classes

- class ConservationLaw

  A conservation law defines the absolute the total amount of a (weighted) sum of states.
- class Constant

  A Constant is a fixed variable in the model with respect to which sensitivites cannot be computed, abbreviated by k
- class Expression

  An Expressions is a recurring elements in symbolic formulas.
- class LogLikelihood

  A LogLikelihood defines the distance between measurements and experiments for a particular observable.
- class ModelQuantity

  Base class for model components.
- class Observable

  An Observable links model simulations to experimental measurements, abbreviated by y
- class ODEExporter

  The ODEExporter class generates AMICI C++ files for ODE model as defined in symbolic expressions.
- class ODEModel

  An ODEModel defines an Ordinay Differential Equation as set of ModelQuantities.
- class Parameter

  A Parameter is a free variable in the model with respect to which sensitivites may be computed, abbreviated by p
- class SigmaY

  A Standard Deviation SigmaY rescales the distance between simulations and measurements when computing residuals, abbreviated by `sigmay`
- class State

  A State variable defines an entity that evolves with time according to the provided time derivative, abbreviated by x
- class TemplateAmici

  Template format used in AMICI (see string.template for more details).

Functions

- def var_in_function_signature (name, varname)

  Checks if the values for a symbolic variable is passed in the signature of a function.
- def getSymbolicDiagonal (matrix)

  Get symbolic matrix with diagonal of matrix `matrix`.
- def applyTemplate (sourceFile, targetFile, templateData)

  Load source file, apply template substitution as provided in templateData and save as targetFile.
- def sanitize_basic_sympy (basic)

  Strips pysb info from the sympy.Basic object.
- def get_function_defition (fun, name)

  Constructs the function definition for a given function.
- def get_function_implementation (fun, name)

  Constructs the function implementation for a given function.
- def remove_typedefs (signature)

  Strips typedef info from a function signature.

Variables

- pysb = None

  pysb import dummy
- dictionary functions

  prototype for generated C++ functions, keys are the names of functions
- list sparse_functions

  list of sparse functions
- list sensi_functions

  list of sensitivity functions
- list multiobs_functions

  list of multiobs functions
- dictionary symbol_to_type

  indicates which type some attributes in ODEModel should have

9.2.1 Detailed Description

!/usr/bin/env python3

9.2.2 Function Documentation

9.2.2.1 var_in_function_signature()

```
def amici.ode_export.var_in_function_signature (
            name,
            varname )
```

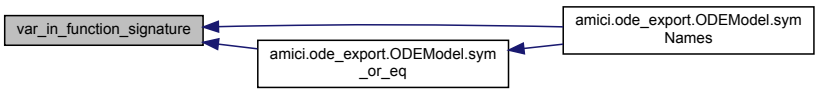
Parameters

name	name of the function **Type**: str
varname	name of the symbolic variable **Type**: str

Returns

Definition at line 287 of file ode_export.py.

Here is the caller graph for this function:



9.2.2.2 getSymbolicDiagonal()

```
def amici.ode_export.getSymbolicDiagonal (
              matrix )
```

Parameters

matrix	Matrix from which to return the diagonal **Type**: symengine.DenseMatrix

Returns

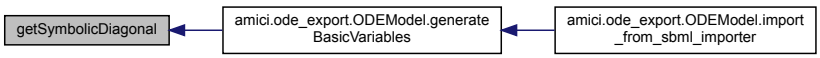
A Symbolic matrix with the diagonal of `matrix`.

Exceptions

Exception	The provided matrix was not square

Definition at line 2634 of file ode_export.py.

Here is the caller graph for this function:



9.2.2.3 applyTemplate()

```
def amici.ode_export.applyTemplate (
            sourceFile,
            targetFile,
            templateData )
```

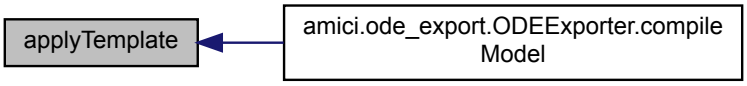
Parameters

sourceFile	relative or absolute path to template file **Type**: str
targetFile	relative or absolute path to output file **Type**: str
templateData	template keywords to substitute (key is template variable without TemplateAmici.delimiter) **Type**: dict

Returns

Definition at line 2670 of file ode_export.py.

Here is the caller graph for this function:



9.2.2.4 sanitize_basic_sympy()

```
def amici.ode_export.sanitize_basic_sympy (
            basic )
```

Parameters

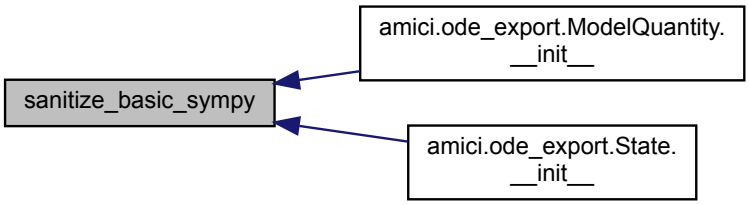
basic	symbolic expression **Type**: sympy.Basic

Returns

sanitized sympy.Basic

Definition at line 2689 of file ode_export.py.

Here is the caller graph for this function:



9.2.2.5 get_function_defition()

```
def amici.ode_export.get_function_defition (
            fun,
            name )
```

Parameters

fun	function name **Type**: str
name	model name **Type**: str

Returns

c++ function definition string

Definition at line 2718 of file ode_export.py.

Here is the caller graph for this function:

9.2.2.6 get_function_implementation()

```
def amici.ode_export.get_function_implementation (
            fun,
            name )
```

Parameters

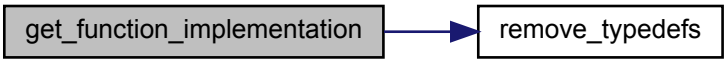
fun	function name **Type**: str
name	model name **Type**: str

Returns

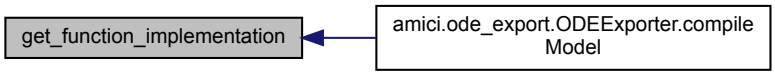
c++ function implementation string

Definition at line 2735 of file ode_export.py.

Here is the call graph for this function:



Here is the caller graph for this function:



9.2.2.7 remove_typedefs()

```
def amici.ode_export.remove_typedefs (
              signature )
```

Parameters

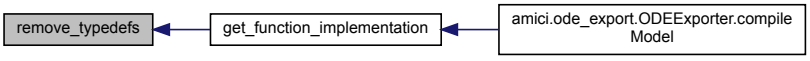
signature	function signature **Type**: str

Returns

string that can be used to construct function calls with the same variable names and ordering as in the function signature

Definition at line 2761 of file ode_export.py.

Here is the caller graph for this function:



9.2.3 Variable Documentation

9.2.3.1 functions

```
dictionary functions
```

signature: defines the argument part of the function signature, input variables should have a const flag

assume_pow_positivity: identifies the functions on which assume_pow_positivity will have an effect when specified during model generation. generally these are functions that are used for solving the ODE, where negative values may negatively affect convergence of the integration algorithm

sparse: specifies whether the result of this function will be stored in sparse format. sparse format means that the function will only return an array of nonzero values and not a full matrix.

Definition at line 40 of file ode_export.py.

9.2.3.2 sparse_functions

```
list sparse_functions
```

Initial value:

```
1 =  [
2     function for function in functions
3     if 'sparse' in functions[function]
4     and functions[function]['sparse']
5 ]
```

Definition at line 256 of file ode_export.py.

9.2.3.3 sensi_functions

```
list sensi_functions
```

Initial value:

```
1 =  [
2     function for function in functions
3     if 'const int ip' in functions[function]['signature']
4     and function is not 'sxdot'
5 ]
```

Definition at line 262 of file ode_export.py.

9.2.3.4 multiobs_functions

```
list multiobs_functions
```

Initial value:

```
1 =  [
2     function for function in functions
3     if 'const int iy' in functions[function]['signature']
4 ]
```

Definition at line 268 of file ode_export.py.

9.2.3.5 symbol_to_type

```
dictionary symbol_to_type
```

Initial value:

```
1 =  {
2     'species': State,
3     'parameter': Parameter,
4     'fixed_parameter': Constant,
5     'observable': Observable,
6     'sigmay': SigmaY,
7     'llhy': LogLikelihood,
8     'expression': Expression,
9 }
```

Definition at line 686 of file ode_export.py.

9.3 amici.plotting Namespace Reference

Plotting related functions.

Functions

- def plotStateTrajectories (rdata, state_indices=None, ax=None)

  Plot state trajectories.
- def plotObservableTrajectories (rdata, observable_indices=None, ax=None)

  Plot observable trajectories.

9.3.1 Function Documentation

9.3.1.1 plotStateTrajectories()

```
def amici.plotting.plotStateTrajectories (
            rdata,
            state_indices = None,
            ax = None )
```

Parameters

rdata	AMICI simulation results as returned by amici.getSimulationResults()
state_indices	Indices of states for which trajectories are to be plotted
ax	matplotlib.axes.Axes instance to plot into

Returns

Definition at line 17 of file plotting.py.

9.3.1.2 plotObservableTrajectories()

```
def amici.plotting.plotObservableTrajectories (
            rdata,
            observable_indices = None,
            ax = None )
```

Parameters

rdata	AMICI simulation results as returned by amici.getSimulationResults()
observable_indices	Indices of observables for which trajectories are to be plotted
ax	matplotlib.axes.Axes instance to plot into

Returns

Definition at line 42 of file plotting.py.

9.4 amici.sbml_import Namespace Reference

The python sbml import module for python.

Classes

- class SBMLException
- class SbmlImporter

  The SbmlImporter class generates AMICI C++ files for a model provided in the Systems Biology Markup Language (SBML).

Functions

- def getRuleVars (rules)

  Extract free symbols in SBML rule formulas.
- def assignmentRules2observables (sbml_model, filter_function=lambda ∗_:True)

  Turn assignment rules into observables.
- def constantSpeciesToParameters (sbml_model)

  Convert constant species in the SBML model to constant parameters.
- def replaceLogAB (x)

  Replace log(a, b) in the given string by ln(b)/ln(a)
- def l2s (inputs)

  transforms an list into list of strings
- def checkLibSBMLErrors (sbml_doc, show_warnings=False)

  Checks the error log in the current self.sbml_doc.

Variables

- dictionary default_symbols

  default dict for symbols

9.4.1 Function Documentation

9.4.1.1 getRuleVars()

```
def amici.sbml_import.getRuleVars (
            rules )
```

Parameters

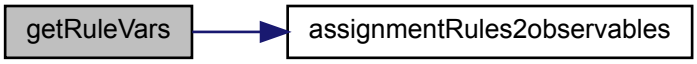
rules	sbml definitions of rules **Type**: list

Returns

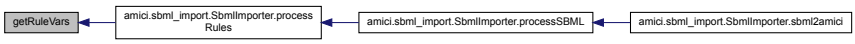
Tuple of free symbolic variables in the formulas all provided rules

Definition at line 975 of file sbml_import.py.

Here is the call graph for this function:



Here is the caller graph for this function:



9.4.1.2 assignmentRules2observables()

```
def amici.sbml_import.assignmentRules2observables (
              sbml_model,
              filter_function = lambda *_: True )
```

Parameters

sbml_model	an sbml Model instance
filter_function	callback function taking assignment variable as input and returning True/False to indicate if the respective rule should be turned into an observable

Returns

A dictionary(observableId:{ 'name': observableName, 'formula': formulaString })

Definition at line 1001 of file sbml_import.py.

Here is the caller graph for this function:

9.4.1.3 constantSpeciesToParameters()

```
def amici.sbml_import.constantSpeciesToParameters (
            sbml_model )
```

Parameters

sbml_model	libsbml model instance

Returns

species IDs that have been turned into constants

Definition at line 1032 of file sbml_import.py.

9.4.1.4 replaceLogAB()

```
def amici.sbml_import.replaceLogAB (
            x )
```

Works for nested parentheses and nested 'log's. This can be used to circumvent the incompatible argument order between symengine (log(x, basis)) and libsbml (log(basis, x)).

Parameters

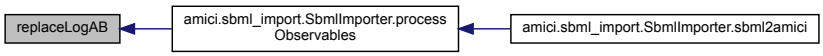
x	string to replace **Type**: str

Returns

string with replaced 'log's

Definition at line 1080 of file sbml_import.py.

Here is the caller graph for this function:



9.4.1.5 l2s()

```
def amici.sbml_import.l2s (
              inputs )
```

Parameters

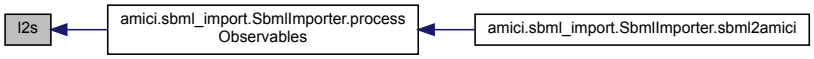
inputs	objects **Type**: list

Returns

list of str(object)

Definition at line 1126 of file sbml_import.py.

Here is the caller graph for this function:



9.4.1.6 checkLibSBMLErrors()

```
def amici.sbml_import.checkLibSBMLErrors (
              sbml_doc,
              show_warnings = False )
```

Parameters

sbml_doc	SBML document **Type**: libsbml.SBMLDocument
show_warnings	display SBML warnings **Type**: bool

Returns

```
raises SBMLException if errors with severity ERROR or FATAL have
```

Exceptions

occurred	

Definition at line 1142 of file sbml_import.py.

9.4.2 Variable Documentation

9.4.2.1 default_symbols

`dictionary default_symbols`

Initial value:

```
1 =  {
2     'species': {},
3     'parameter': {},
4     'fixed_parameter': {},
5     'observable': {},
6     'expression': {},
7     'sigmay': {},
8     'my': {},
9     'llhy': {},
10 }
```

Definition at line 17 of file sbml_import.py.

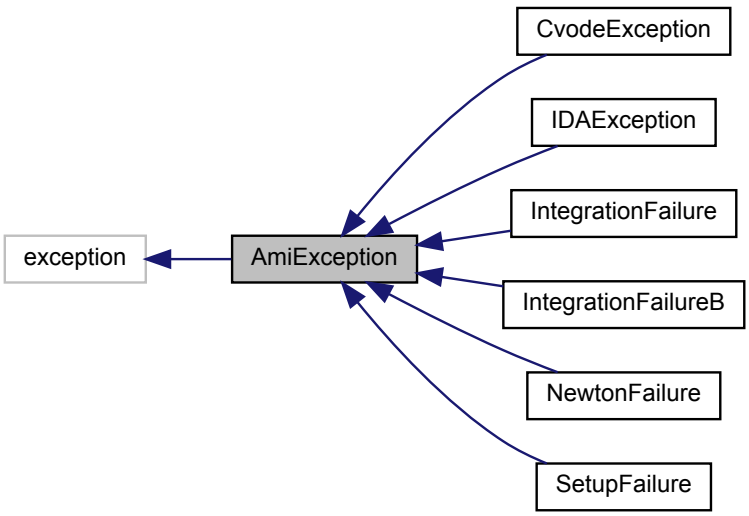
10 Class Documentation

10.1 AmiException Class Reference

amici exception handler class

`#include <exception.h>`

Inheritance diagram for AmiException:



Public Member Functions

- AmiException (char const ∗fmt,...)
- AmiException (const AmiException &old)
- const char ∗ what () const throw ()
- const char ∗ getBacktrace () const
- void storeBacktrace (const int nMaxFrames)

10.1.1 Detailed Description

has a printf style interface to allow easy generation of error messages

Definition at line 29 of file exception.h.

10.1.2 Constructor & Destructor Documentation

10.1.2.1 AmiException() [1/2]

```
AmiException (
            char const * fmt,
             ...  )
```

constructor with printf style interface

Parameters

fmt	error message with printf format
...	printf formating variables

Definition at line 31 of file exception.h.

Here is the call graph for this function:

10.1.2.2 AmiException() [2/2]

```
AmiException (
            const AmiException & old )
```

copy constructor

Parameters

old	object to copy from

Definition at line 43 of file exception.h.

10.1.3 Member Function Documentation

10.1.3.1 what()

```
const char* what ( ) const throw )
```

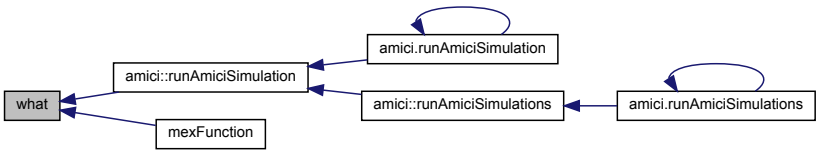
override of default error message function

Returns

msg error message

Definition at line 54 of file exception.h.

Here is the caller graph for this function:



10.1.3.2 getBacktrace()

```
const char* getBacktrace ( ) const
```

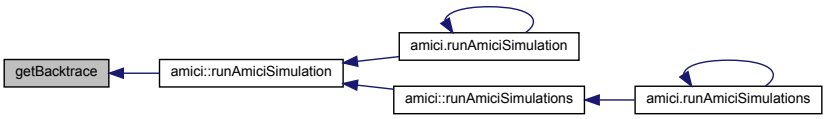
returns the stored backtrace

Returns

trace backtrace

Definition at line 61 of file exception.h.

Here is the caller graph for this function:



10.1.3.3 storeBacktrace()

```
void storeBacktrace (
            const int nMaxFrames )
```

stores the current backtrace

Parameters

nMaxFrames	number of frams to go back in stacktrace

Definition at line 68 of file exception.h.

Here is the caller graph for this function:

10.2 AmiVector Class Reference

```
#include <vector.h>
```

Public Member Functions

- AmiVector (const long int length)
- AmiVector (std::vector< realtype > rvec)
- AmiVector (const AmiVector &vold)
- AmiVector & operator= (AmiVector const &other)
- realtype * data ()
- const realtype * data () const
- N_Vector getNVector () const
- std::vector< realtype > const & getVector () const
- int getLength () const
- void reset ()
- void minus ()
- void set (realtype val)
- realtype & operator[ ] (int pos)
- realtype & at (int pos)
- const realtype & at (int pos) const

10.2.1 Detailed Description

AmiVector class provides a generic interface to the NVector_Serial struct

Definition at line 12 of file vector.h.

10.2.2 Constructor & Destructor Documentation

10.2.2.1 AmiVector() [1/3]

```
AmiVector (
            const long int length )
```

Creates an std::vector<realtype> and attaches the data pointer to a newly created N_Vector_Serial. Using N↩_VMake_Serial ensures that the N_Vector module does not try to deallocate the data vector when calling N_V↩Destroy_Serial

Parameters

length	number of elements in vector

Returns

new AmiVector instance

Definition at line 24 of file vector.h.

10.2.2.2 AmiVector() [2/3]

```
AmiVector (
            std::vector< realtype > rvec )
```

constructor from std::vector, copies data from std::vector and constructs an nvec that points to the data

Parameters

rvec	vector from which the data will be copied

Returns

new AmiVector instance

Definition at line 35 of file vector.h.

10.2.2.3 AmiVector() [3/3]

```
AmiVector (
            const AmiVector & vold )
```

copy constructor

Parameters

vold	vector from which the data will be copied

Definition at line 44 of file vector.h.

10.2.3 Member Function Documentation

10.2.3.1 operator=()

```
AmiVector& operator= (
            AmiVector const & other )
```

copy-move assignment operator

Parameters

other	right hand side

Returns

left hand side

Definition at line 53 of file vector.h.

10.2.3.2 data() [1/2]

```
realtype* data ( )
```

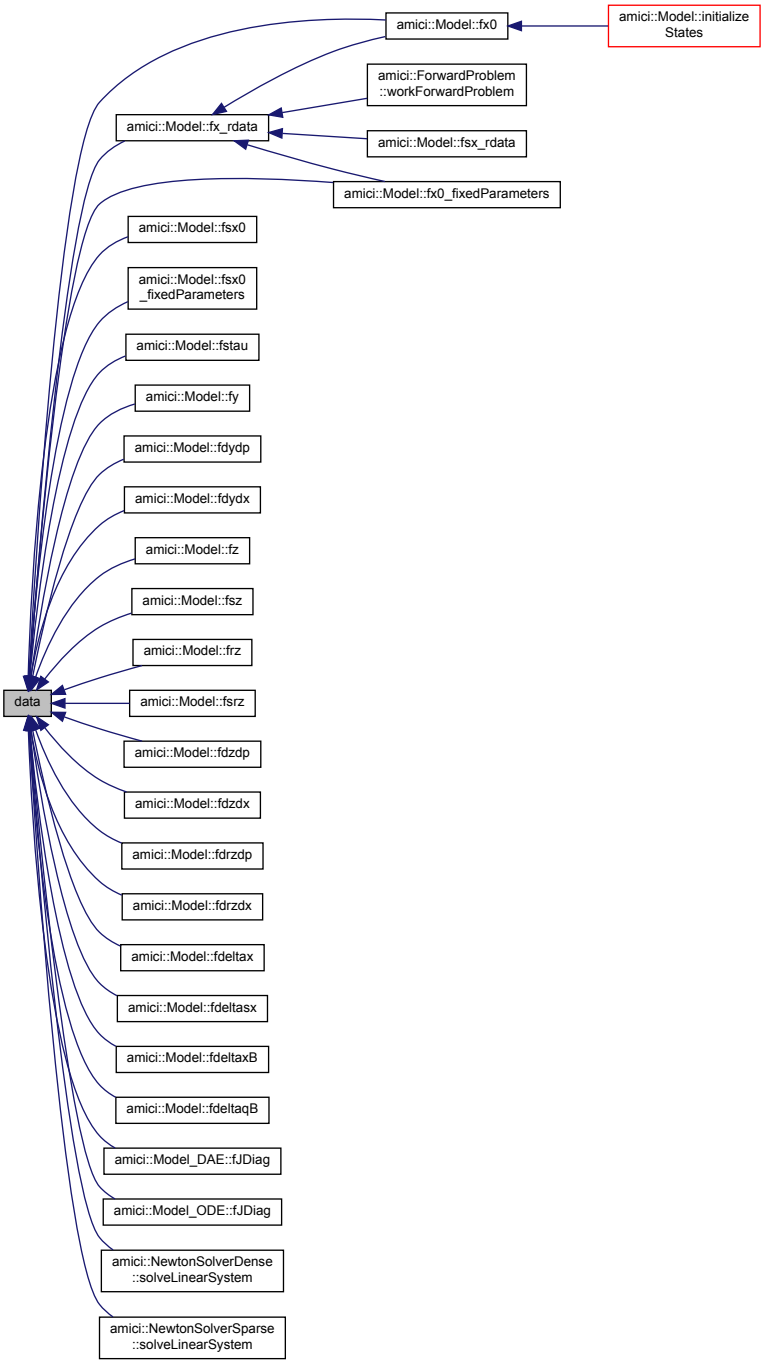
data accessor

Returns

pointer to data array

Definition at line 64 of file vector.h.

Here is the caller graph for this function:



10.2.3.3 data() [2/2]

```
const realtype* data ( ) const
```

const data accessor

Returns

const pointer to data array

Definition at line 71 of file vector.h.

10.2.3.4 getNVector()

```
N_Vector getNVector ( ) const
```

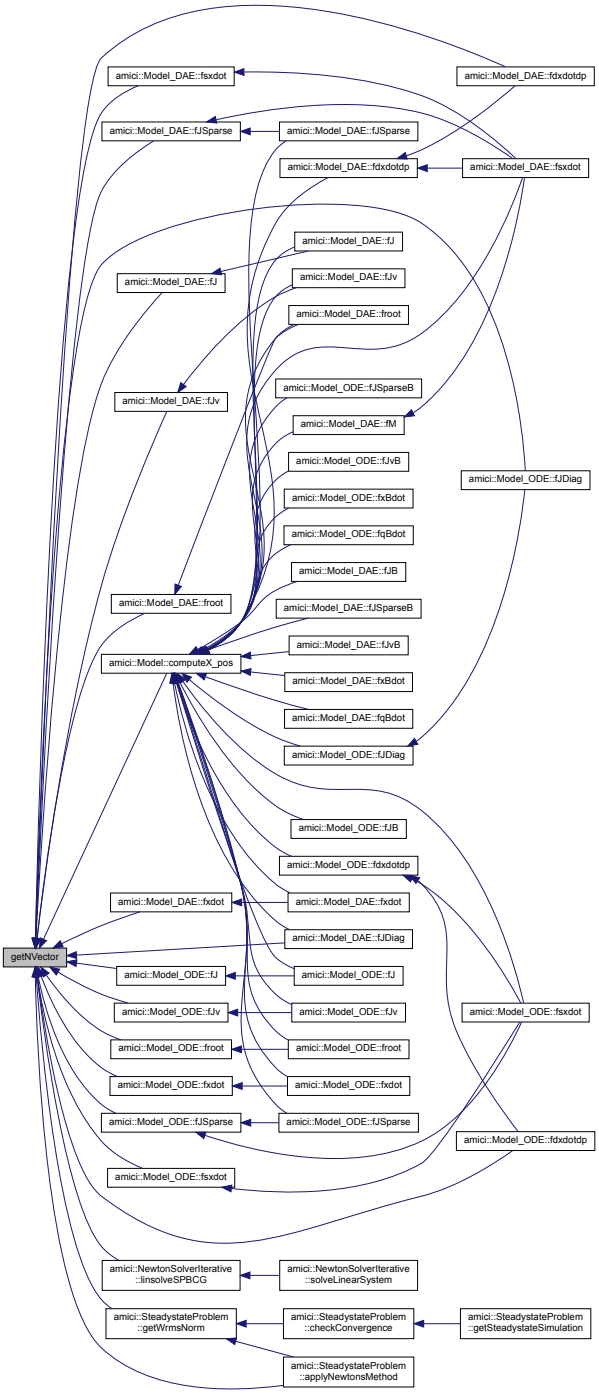
N_Vector accessor

Returns

N_Vector

Definition at line 78 of file vector.h.

Here is the caller graph for this function:



10.2.3.5 getVector()

```
std::vector<realtype> const& getVector ( ) const
```

Vector accessor

Returns

Vector

Definition at line 85 of file vector.h.

10.2.3.6 getLength()

```
int getLength ( ) const
```

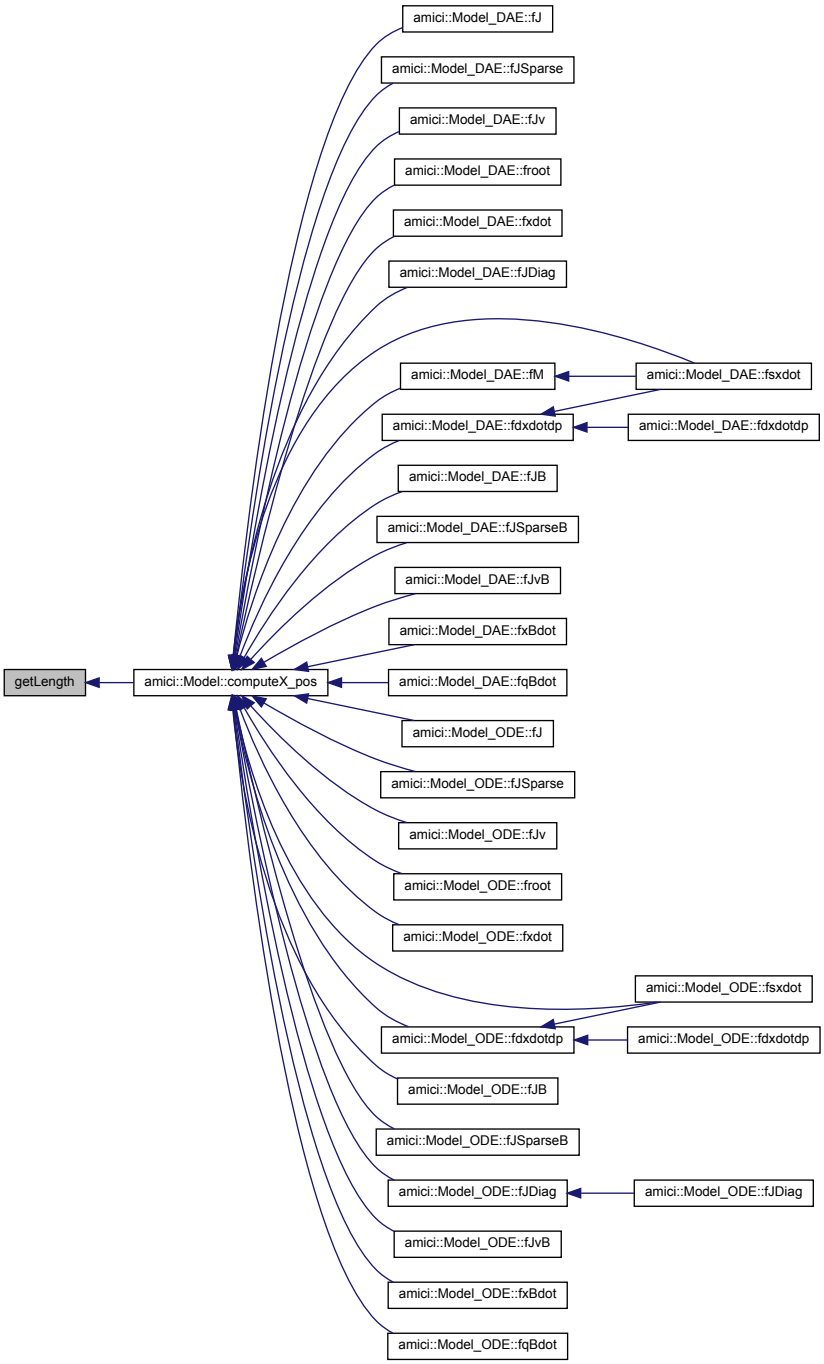
returns the length of the vector

Returns

length

Definition at line 92 of file vector.h.

Here is the caller graph for this function:



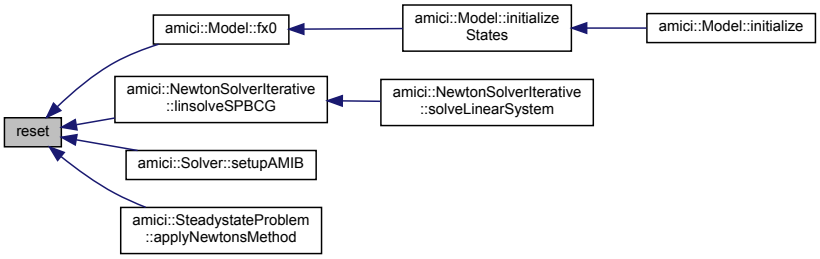
10.2.3.7 reset()

```
void reset ( )
```

resets the Vector by filling with zero values

Definition at line 98 of file vector.h.

Here is the caller graph for this function:



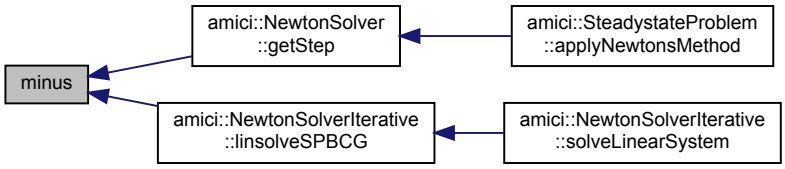
10.2.3.8 minus()

```
void minus ( )
```

changes the sign of data elements

Definition at line 104 of file vector.h.

Here is the caller graph for this function:



10.2.3.9 set()

```
void set (
            realtype val )
```

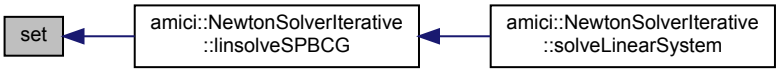
sets all data elements to a specific value

Parameters

val	value for data elements

Definition at line 113 of file vector.h.

Here is the caller graph for this function:



10.2.3.10 operator[]()

```
realtype& operator[] (
            int pos )
```

accessor to data elements of the vector

Parameters

pos	index of element

Returns

element

Definition at line 121 of file vector.h.

10.2.3.11 at() [1/2]

```
realtype& at (
            int pos )
```

accessor to data elements of the vector

Parameters

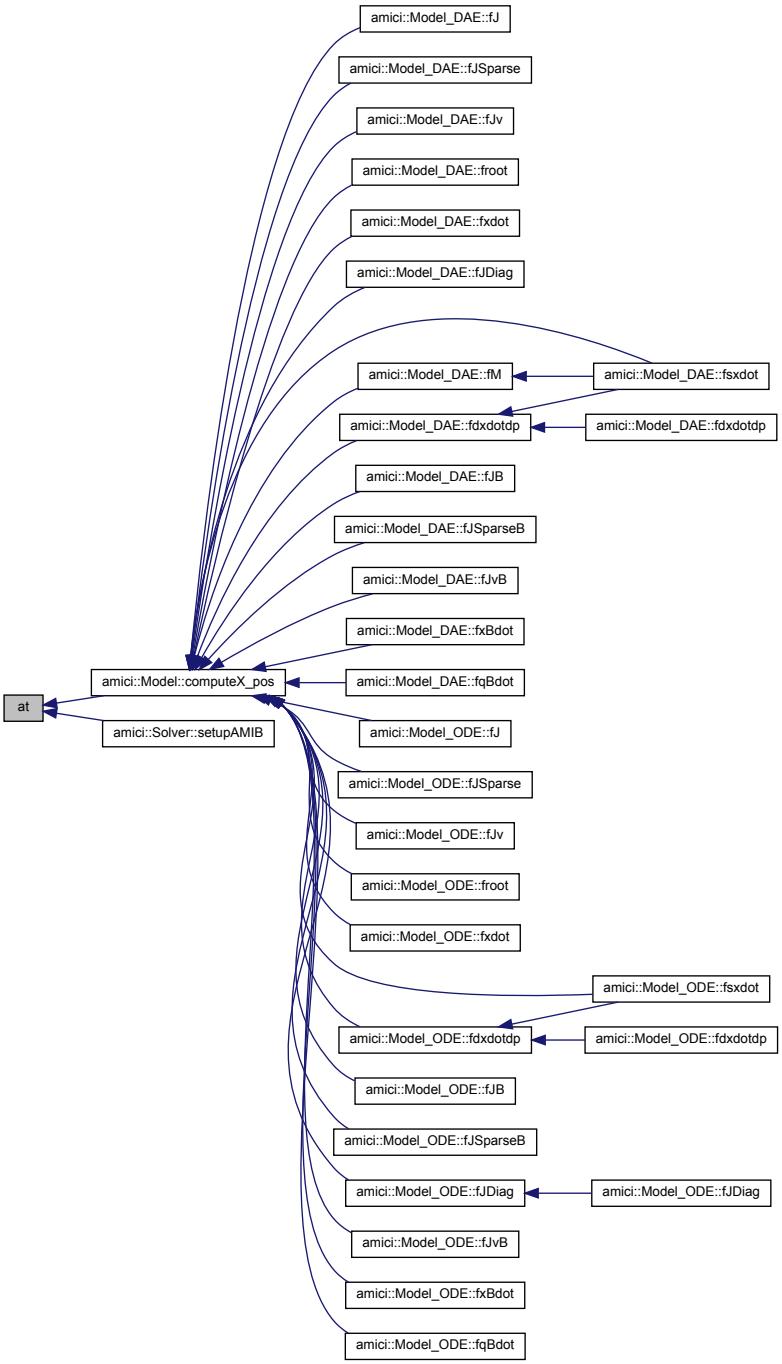
pos	index of element

Returns

element

Definition at line 129 of file vector.h.

Here is the caller graph for this function:



10.2.3.12 at() [2/2]

```
const realtype& at (
            int pos ) const
```

accessor to data elements of the vector

Parameters

pos	index of element

Returns

element

Definition at line 137 of file vector.h.

10.3 AmiVectorArray Class Reference

```
#include <vector.h>
```

Public Member Functions

- AmiVectorArray (long int length_inner, long int length_outer)
- AmiVectorArray (const AmiVectorArray &vaold)
- realtype ∗ data (int pos)
- const realtype ∗ data (int pos) const
- realtype & at (int ipos, int jpos)
- const realtype & at (int ipos, int jpos) const
- N_Vector ∗ getNVectorArray ()
- N_Vector getNVector (int pos)
- AmiVector & operator[ ] (int pos)
- const AmiVector & operator[ ] (int pos) const
- int getLength () const
- void reset ()
- void flatten_to_vector (std::vector< realtype > &vec) const

10.3.1 Detailed Description

AmiVectorArray class. provides a generic interface to arrays of NVector_Serial structs

Definition at line 157 of file vector.h.

10.3.2 Constructor & Destructor Documentation

10.3.2.1 AmiVectorArray() [1/2]

```
AmiVectorArray (
            long int length_inner,
            long int length_outer )
```

creates an std::vector<realype> and attaches the data pointer to a newly created N_VectorArray using Clone↩ VectorArrayEmpty ensures that the N_Vector module does not try to deallocate the data vector when calling N_V↩ DestroyVectorArray_Serial

Parameters

length_inner	length of vectors
length_outer	number of vectors

Returns

New AmiVectorArray instance

Definition at line 168 of file vector.h.

10.3.2.2 AmiVectorArray() [2/2]

```
AmiVectorArray (
            const AmiVectorArray & vaold )
```

copy constructor

Parameters

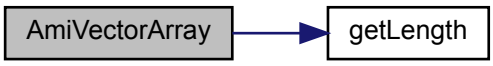
vaold	object to copy from

Returns

new AmiVectorArray instance

Definition at line 182 of file vector.h.

Here is the call graph for this function:



10.3.3 Member Function Documentation

10.3.3.1 data() [1/2]

```
realtype* data (
            int pos )
```

accessor to data of AmiVector elements

Parameters

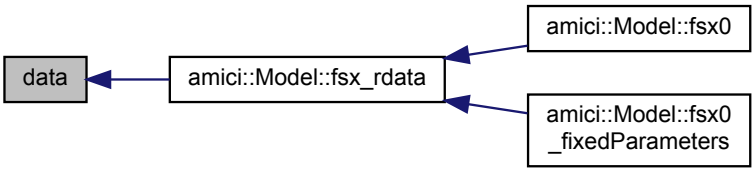
pos	index of AmiVector

Returns

pointer to data array

Definition at line 193 of file vector.h.

Here is the caller graph for this function:



10.3.3.2 data() [2/2]

```
const realtype* data (
            int pos ) const
```

const accessor to data of AmiVector elements

Parameters

pos	index of AmiVector

Returns

const pointer to data array

Definition at line 201 of file vector.h.

10.3.3.3 at() [1/2]

```
realtype& at (
            int ipos,
            int jpos )
```

accessor to elements of AmiVector elements

Parameters

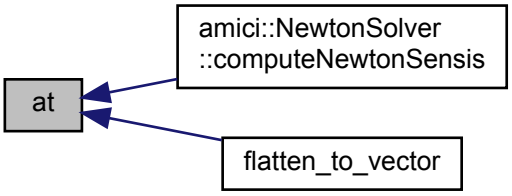
ipos	inner index in AmiVector
jpos	outer index in AmiVectorArray

Returns

element

Definition at line 210 of file vector.h.

Here is the caller graph for this function:



10.3.3.4 at() [2/2]

```
const realtype& at (
            int ipos,
            int jpos ) const
```

accessor to elements of AmiVector elements

Parameters

ipos	inner index in AmiVector
jpos	outer index in AmiVectorArray

Returns

element

Definition at line 219 of file vector.h.

10.3.3.5 getNVectorArray()

```
N_Vector* getNVectorArray ( )
```

accessor to NVectorArray

Returns

N_VectorArray

Definition at line 226 of file vector.h.

10.3.3.6 getNVector()

```
N_Vector getNVector (
            int pos )
```

accessor to NVector element

Parameters

pos	index of corresponding AmiVector

Returns

N_Vector

Definition at line 234 of file vector.h.

10.3.3.7 operator[]() [1/2]

```
AmiVector& operator[] (
            int pos )
```

accessor to AmiVector elements

Parameters

pos	index of AmiVector

Returns

AmiVector

Definition at line 242 of file vector.h.

10.3.3.8 operator[]() [2/2]

```
const AmiVector& operator[] (
            int pos ) const
```

const accessor to AmiVector elements

Parameters

pos	index of AmiVector

Returns

const AmiVector

Definition at line 250 of file vector.h.

10.3.3.9 getLength()

```
int getLength ( ) const
```

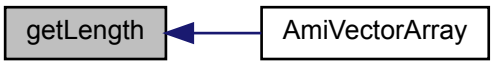
length of AmiVectorArray

Returns

length

Definition at line 257 of file vector.h.

Here is the caller graph for this function:



10.3.3.10 reset()

```
void reset ( )
```

resets every AmiVector in AmiVectorArray

Definition at line 262 of file vector.h.

10.3.3.11 flatten_to_vector()

```
void flatten_to_vector (
            std::vector< realtype > & vec ) const
```

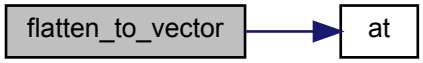
flattens the AmiVectorArray to a vector in row-major format

Parameters

vec	vector into which the AmiVectorArray will be flattened. Must have length equal to number of elements.

Definition at line 271 of file vector.h.

Here is the call graph for this function:



10.4 BackwardProblem Class Reference

class to solve backwards problems.

```
#include <backwardproblem.h>
```

Public Member Functions

- void workBackwardProblem ()
- BackwardProblem (const ForwardProblem *fwd)
- realtype gett () const
- int getwhich () const
- int * getwhichptr ()
- AmiVector * getxBptr ()
- AmiVector * getxQBptr ()
- AmiVector * getdxBptr ()
- std::vector< realtype > const & getdJydx () const

10.4.1 Detailed Description

solves the backwards problem for adjoint sensitivity analysis and handles events and data-points

Definition at line 23 of file backwardproblem.h.

10.4.2 Constructor & Destructor Documentation

10.4.2.1 BackwardProblem()

```
BackwardProblem (
            const ForwardProblem * fwd )
```

Construct backward problem from forward problem

Parameters

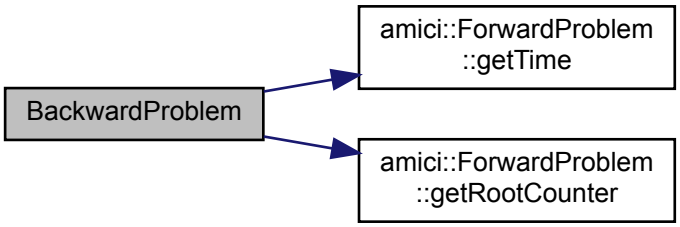
fwd	pointer to corresponding forward problem

Returns

new BackwardProblem instance

Definition at line 18 of file backwardproblem.cpp.

Here is the call graph for this function:



10.4.3 Member Function Documentation

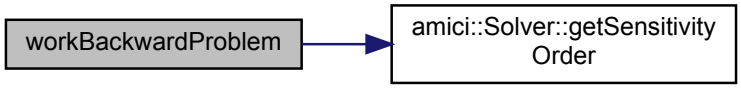
10.4.3.1 workBackwardProblem()

```
void workBackwardProblem ( )
```

workBackwardProblem solves the backward problem. if adjoint sensitivities are enabled this will also compute sensitivies workForwardProblem should be called before this is function is called

Definition at line 42 of file backwardproblem.cpp.

Here is the call graph for this function:



10.4.3.2 gett()

```
realtype gett ( ) const
```

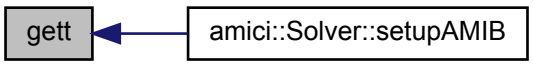
accessor for t

Returns

t

Definition at line 32 of file backwardproblem.h.

Here is the caller graph for this function:



10.4.3.3 getwhich()

```
int getwhich ( ) const
```

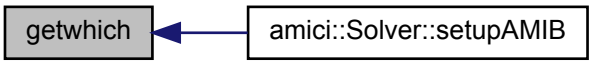
accessor for which

Returns

which

Definition at line 39 of file backwardproblem.h.

Here is the caller graph for this function:



10.4.3.4 getwhichptr()

```
int* getwhichptr ( )
```

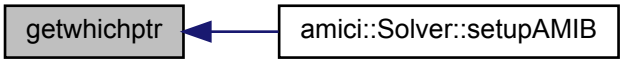
accessor for pointer to which

Returns

which

Definition at line 46 of file backwardproblem.h.

Here is the caller graph for this function:



10.4.3.5 getxBptr()

```
AmiVector* getxBptr ( )
```

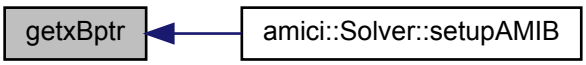
accessor for pointer to xB

Returns

&xB

Definition at line 53 of file backwardproblem.h.

Here is the caller graph for this function:



10.4.3.6 getxQBptr()

```
AmiVector* getxQBptr ( )
```

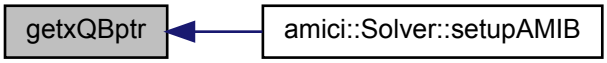
accessor for pointer to xQB

Returns

&xQB

Definition at line 60 of file backwardproblem.h.

Here is the caller graph for this function:



10.4.3.7 getdxBptr()

```
AmiVector* getdxBptr ( )
```

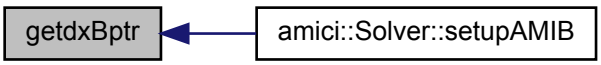
accessor for pointer to dxB

Returns

&dxB

Definition at line 67 of file backwardproblem.h.

Here is the caller graph for this function:



10.4.3.8 getdJydx()

```
std::vector<realtype> const& getdJydx ( ) const
```

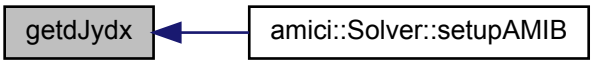
accessor for dJydx

Returns

dJydx

Definition at line 74 of file backwardproblem.h.

Here is the caller graph for this function:

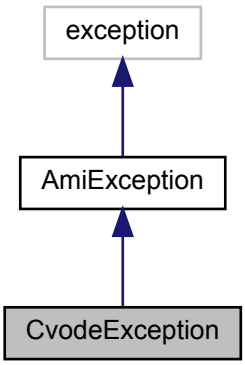


10.5 CvodeException Class Reference

cvode exception handler class

```
#include <exception.h>
```

Inheritance diagram for CvodeException:



Public Member Functions

- CvodeException (const int error_code, const char *function)

10.5.1 Detailed Description

Definition at line 117 of file exception.h.

10.5.2 Constructor & Destructor Documentation

10.5.2.1 CvodeException()

```
CvodeException (
            const int error_code,
            const char * function )
```

constructor

Parameters

error_code	error code returned by cvode function
function	cvode function name

Definition at line 123 of file exception.h.

10.6 ExpData Class Reference

ExpData carries all information about experimental or condition-specific data.

```
#include <edata.h>
```

Public Member Functions

- ExpData ()
- ExpData (const ExpData &)=default
- ExpData (int nytrue, int nztrue, int nmaxevent)
- ExpData (int nytrue, int nztrue, int nmaxevent, std::vector< realtype > ts)
- ExpData (int nytrue, int nztrue, int nmaxevent, std::vector< realtype > ts, std::vector< realtype > observedData, std::vector< realtype > observedDataStdDev, std::vector< realtype > observedEvents, std::vector< realtype > observedEventsStdDev)
- ExpData (const Model &model)
- ExpData (const ReturnData &rdata, realtype sigma_y, realtype sigma_z)
- ExpData (const ReturnData &rdata, std::vector< realtype > sigma_y, std::vector< realtype > sigma_z)
- int nytrue () const
- int nztrue () const
- int nmaxevent () const
- int nt () const
- void setTimepoints (const std::vector< realtype > &ts)
- std::vector< realtype > const & getTimepoints () const
- realtype getTimepoint (int it) const
- void setObservedData (const std::vector< realtype > &observedData)

- void setObservedData (const std::vector< realtype > &observedData, int iy)
- bool isSetObservedData (int it, int iy) const
- std::vector< realtype > const & getObservedData () const
- const realtype * getObservedDataPtr (int it) const
- void setObservedDataStdDev (const std::vector< realtype > &observedDataStdDev)
- void setObservedDataStdDev (const realtype stdDev)
- void setObservedDataStdDev (const std::vector< realtype > &observedDataStdDev, int iy)
- void setObservedDataStdDev (const realtype stdDev, int iy)
- bool isSetObservedDataStdDev (int it, int iy) const
- std::vector< realtype > const & getObservedDataStdDev () const
- const realtype * getObservedDataStdDevPtr (int it) const
- void setObservedEvents (const std::vector< realtype > &observedEvents)
- void setObservedEvents (const std::vector< realtype > &observedEvents, int iz)
- bool isSetObservedEvents (int ie, int iz) const
- std::vector< realtype > const & getObservedEvents () const
- const realtype * getObservedEventsPtr (int ie) const
- void setObservedEventsStdDev (const std::vector< realtype > &observedEventsStdDev)
- void setObservedEventsStdDev (const realtype stdDev)
- void setObservedEventsStdDev (const std::vector< realtype > &observedEventsStdDev, int iz)
- void setObservedEventsStdDev (const realtype stdDev, int iz)
- bool isSetObservedEventsStdDev (int ie, int iz) const
- std::vector< realtype > const & getObservedEventsStdDev () const
- const realtype * getObservedEventsStdDevPtr (int ie) const

Public Attributes

- std::vector< realtype > fixedParameters
- std::vector< realtype > fixedParametersPreequilibration
- std::vector< realtype > fixedParametersPresimulation
- realtype t_presim = 0

  duration of pre-simulation if this is > 0, presimualation will be performed from (model->t0 - t_presim) to model->t0 using the fixedParameters in fixedParametersPresimulation

Protected Member Functions

- void checkDataDimension (std::vector< realtype > input, const char *fieldname) const
- void checkEventsDimension (std::vector< realtype > input, const char *fieldname) const
- void checkSigmaPositivity (std::vector< realtype > sigmaVector, const char *vectorName) const
- void checkSigmaPositivity (realtype sigma, const char *sigmaName) const

Protected Attributes

- int nytrue_
- int nztrue_
- int nmaxevent_
- std::vector< realtype > ts
- std::vector< realtype > observedData
- std::vector< realtype > observedDataStdDev
- std::vector< realtype > observedEvents
- std::vector< realtype > observedEventsStdDev

10.6.1 Detailed Description

Definition at line 14 of file edata.h.

10.6.2 Constructor & Destructor Documentation

10.6.2.1 ExpData() [1/8]

```
ExpData ( )
```

default constructor

Definition at line 14 of file edata.cpp.

10.6.2.2 ExpData() [2/8]

```
ExpData (
            const ExpData &  )  [default]
```

default copy constructor, needs to be declared to be generated in swig

10.6.2.3 ExpData() [3/8]

```
ExpData (
            int nytrue,
            int nztrue,
            int nmaxevent )
```

constructor that only initializes dimensions

Parameters

nytrue	
nztrue	
nmaxevent	

Definition at line 16 of file edata.cpp.

10.6.2.4 ExpData() [4/8]

```
ExpData (
            int nytrue,
            int nztrue,
            int nmaxevent,
            std::vector< realtype > ts )
```

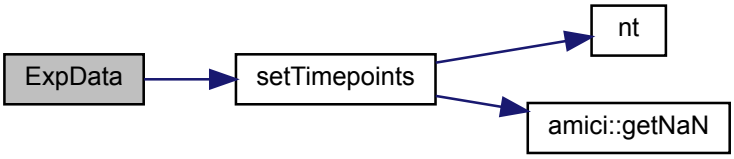
constructor that initializes timepoints from vectors

Parameters

nytrue	(dimension: scalar)
nztrue	(dimension: scalar)
nmaxevent	(dimension: scalar)
ts	(dimension: nt)

Definition at line 21 of file edata.cpp.

Here is the call graph for this function:



10.6.2.5 ExpData() [5/8]

```
ExpData (
            int nytrue,
            int nztrue,
            int nmaxevent,
            std::vector< realtype > ts,
            std::vector< realtype > observedData,
            std::vector< realtype > observedDataStdDev,
            std::vector< realtype > observedEvents,
            std::vector< realtype > observedEventsStdDev )
```

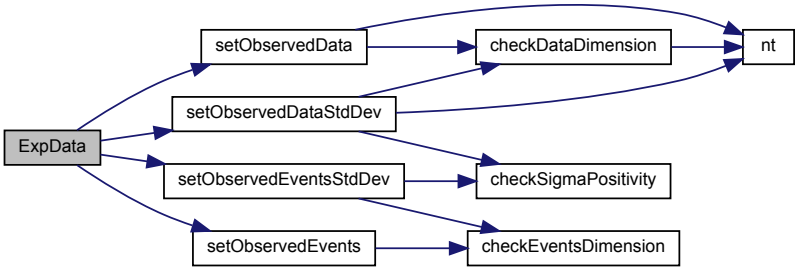
constructor that initializes timepoints and data from vectors

Parameters

nytrue	(dimension: scalar)
nztrue	(dimension: scalar)
nmaxevent	(dimension: scalar)
ts	(dimension: nt)
observedData	(dimension: nt x nytrue, row-major)
observedDataStdDev	(dimension: nt x nytrue, row-major)
observedEvents	(dimension: nmaxevent x nztrue, row-major)
observedEventsStdDev	(dimension: nmaxevent x nztrue, row-major)

Definition at line 28 of file edata.cpp.

Here is the call graph for this function:



10.6.2.6 ExpData() [6/8]

```
ExpData (
            const Model & model )
```

constructor that initializes with Model

Parameters

model	pointer to model specification object

Definition at line 42 of file edata.cpp.

10.6.2.7 ExpData() [7/8]

```
ExpData (
            const ReturnData & rdata,
            realtype sigma_y,
            realtype sigma_z )
```

constructor that initializes with returnData, adds

Parameters

rdata	return data pointer with stored simulation results
sigma↩ _y	scalar standard deviations for all observables
sigma↩ _z	scalar standard deviations for all event observables

Definition at line 48 of file edata.cpp.

10.6.2.8 ExpData() [8/8]

```
ExpData (
            const ReturnData & rdata,
            std::vector< realtype > sigma_y,
            std::vector< realtype > sigma_z )
```

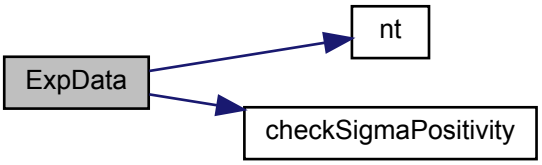
constructor that initializes with returnData, adds

Parameters

rdata	return data pointer with stored simulation results
sigma↩ _y	vector of standard deviations for observables (dimension: nytrue or nt x nytrue, row-major)
sigma↩ _z	vector of standard deviations for event observables (dimension: nztrue or nmaxevent x nztrue, row-major)

Definition at line 53 of file edata.cpp.

Here is the call graph for this function:



10.6.3 Member Function Documentation

10.6.3.1 nytrue()

```
int nytrue ( ) const
```

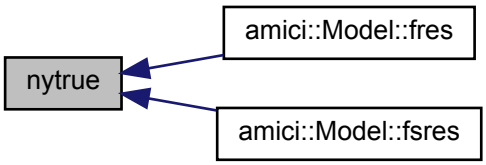
number of observables of the non-augmented model

Returns

number of observables of the non-augmented model

Definition at line 290 of file edata.cpp.

Here is the caller graph for this function:



10.6.3.2 nztrue()

```
int nztrue ( ) const
```

number of event observables of the non-augmented model

Returns

number of event observables of the non-augmented model

Definition at line 295 of file edata.cpp.

10.6.3.3 nmaxevent()

```
int nmaxevent ( ) const
```

maximal number of events to track

Returns

maximal number of events to track

Definition at line 300 of file edata.cpp.

10.6.3.4 nt()

```
int nt ( ) const
```

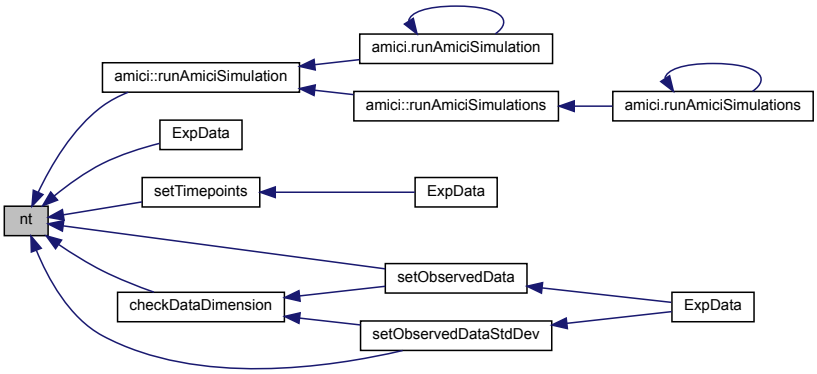
number of timepoints

Returns

number of timepoints

Definition at line 102 of file edata.cpp.

Here is the caller graph for this function:



10.6.3.5 setTimepoints()

```
void setTimepoints (
            const std::vector< realtype > & ts )
```

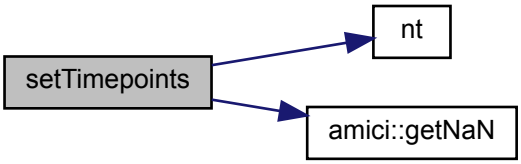
set function that copies data from input to ExpData::ts

Parameters

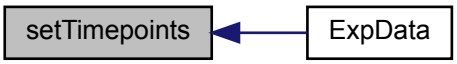
ts	timepoints

Definition at line 89 of file edata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.6.3.6 getTimepoints()

```
std::vector< realtype > const & getTimepoints ( ) const
```

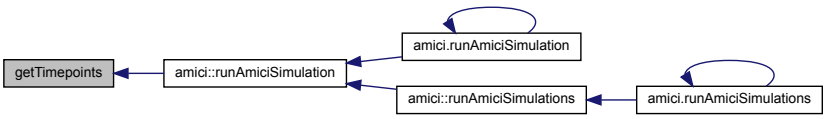
get function that copies data from ExpData::ts to output

Returns

ExpData::ts

Definition at line 98 of file edata.cpp.

Here is the caller graph for this function:



10.6.3.7 getTimepoint()

```
realtype getTimepoint (
            int it ) const
```

get function that returns timepoint at index

Parameters

it	timepoint index

Returns

timepoint timepoint at index

Definition at line 106 of file edata.cpp.

10.6.3.8 setObservedData() [1/2]

```
void setObservedData (
            const std::vector< realtype > & observedData )
```

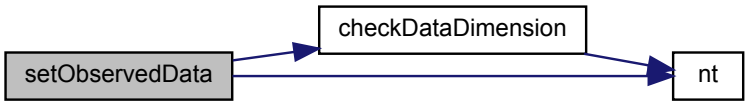
set function that copies data from input to ExpData::my

Parameters

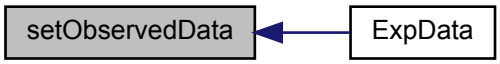
observedData	observed data (dimension: nt x nytrue, row-major)

Definition at line 110 of file edata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.6.3.9 setObservedData() [2/2]

```
void setObservedData (
            const std::vector< realtype > & observedData,
            int iy )
```

set function that copies observed data for specific observable

Parameters

observedData	observed data (dimension: nt)
iy	oberved data index

Definition at line 119 of file edata.cpp.

Here is the call graph for this function:

10.6.3.10 isSetObservedData()

```
bool isSetObservedData (
            int it,
            int iy ) const
```

get function that checks whether data at specified indices has been set

Parameters

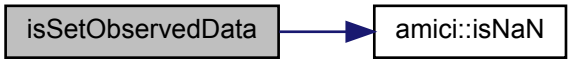
it	time index
iy	observable index

Returns

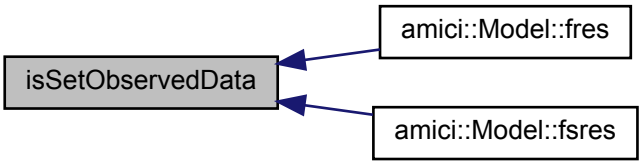
boolean specifying if data was set

Definition at line 127 of file edata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.6.3.11 getObservedData()

```
std::vector< realtype > const & getObservedData ( ) const
```

get function that copies data from ExpData::observedData to output

Returns

observed data (dimension: nt x nytrue, row-major)

Definition at line 131 of file edata.cpp.

10.6.3.12 getObservedDataPtr()

```
const realtype * getObservedDataPtr (
            int it ) const
```

get function that returns a pointer to observed data at index

Parameters

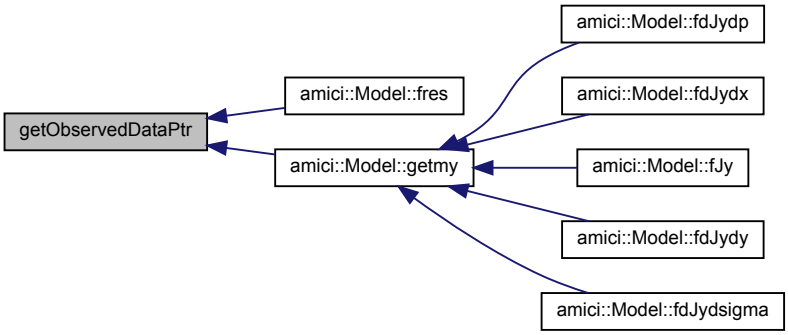
it	timepoint index

Returns

pointer to observed data at index (dimension: nytrue)

Definition at line 135 of file edata.cpp.

Here is the caller graph for this function:



10.6.3.13 setObservedDataStdDev() [1/4]

```
void setObservedDataStdDev (
            const std::vector< realtype > & observedDataStdDev )
```

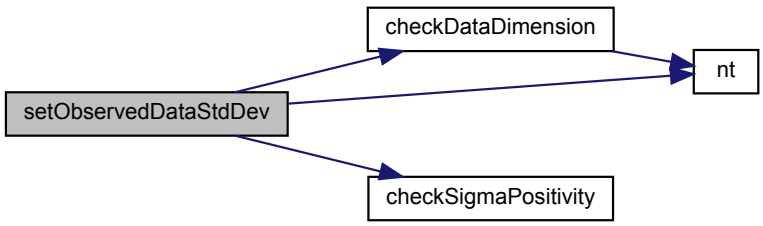
set function that copies data from input to ExpData::observedDataStdDev

Parameters

observedDataStdDev	standard deviation of observed data (dimension: nt x nytrue, row-major)

Definition at line 142 of file edata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.6.3.14 setObservedDataStdDev() [2/4]

```
void setObservedDataStdDev (
            const realtype stdDev )
```

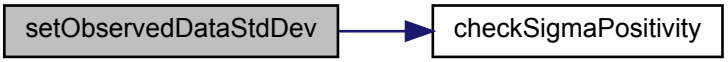
set function that sets all ExpData::observedDataStdDev to the input value

Parameters

stdDev	standard deviation (dimension: scalar)

Definition at line 152 of file edata.cpp.

Here is the call graph for this function:



10.6.3.15 setObservedDataStdDev() [3/4]

```
void setObservedDataStdDev (
            const std::vector< realtype > & observedDataStdDev,
            int iy )
```

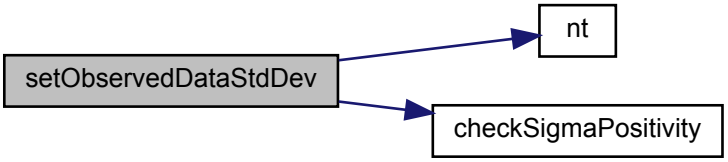
set function that copies standard deviation of observed data for specific observable

Parameters

observedDataStdDev	standard deviation of observed data (dimension: nt)
iy	observed data index

Definition at line 157 of file edata.cpp.

Here is the call graph for this function:



10.6.3.16 setObservedDataStdDev() [4/4]

```
void setObservedDataStdDev (
            const realtype stdDev,
            int iy )
```

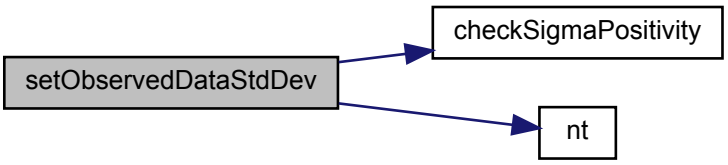
set function that sets all standard deviation of a specific observable to the input value

Parameters

stdDev	standard deviation (dimension: scalar)
iy	observed data index

Definition at line 166 of file edata.cpp.

Here is the call graph for this function:



10.6.3.17 isSetObservedDataStdDev()

```
bool isSetObservedDataStdDev (
            int it,
            int iy ) const
```

get function that checks whether standard deviation of data at specified indices has been set

Parameters

it	time index
iy	observable index

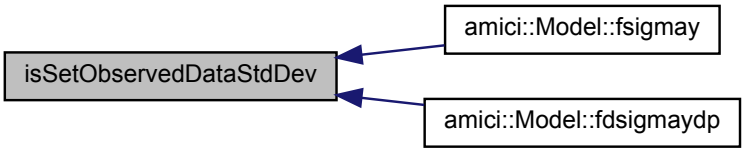
Returns

boolean specifying if standard deviation of data was set

Definition at line 172 of file edata.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



10.6.3.18 getObservedDataStdDev()

```
std::vector< realtype > const & getObservedDataStdDev ( ) const
```

get function that copies data from ExpData::observedDataStdDev to output

Returns

standard deviation of observed data

Definition at line 176 of file edata.cpp.

10.6.3.19 getObservedDataStdDevPtr()

```
const realtype * getObservedDataStdDevPtr (
            int it ) const
```

get function that returns a pointer to standard deviation of observed data at index

Parameters

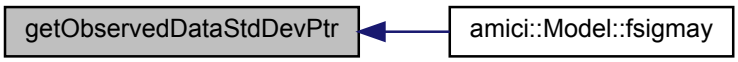
it	timepoint index

Returns

pointer to standard deviation of observed data at index

Definition at line 180 of file edata.cpp.

Here is the caller graph for this function:



10.6.3.20 setObservedEvents() [1/2]

```
void setObservedEvents (
            const std::vector< realtype > & observedEvents )
```

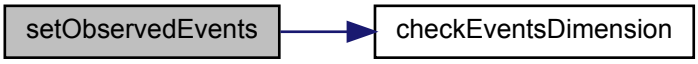
set function that copies observed event data from input to ExpData::observedEvents

Parameters

observedEvents	observed data (dimension: nmaxevent x nztrue, row-major)

Definition at line 187 of file edata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.6.3.21 setObservedEvents() [2/2]

```
void setObservedEvents (
            const std::vector< realtype > & observedEvents,
            int iz )
```

set function that copies observed event data for specific event observable

Parameters

observedEvents	observed data (dimension: nmaxevent)
iz	observed event data index

Definition at line 196 of file edata.cpp.

10.6.3.22 isSetObservedEvents()

```
bool isSetObservedEvents (
            int ie,
            int iz ) const
```

get function that checks whether event data at specified indices has been set

Parameters

ie	event index
iz	event observable index

Returns

boolean specifying if data was set

Definition at line 205 of file edata.cpp.

Here is the call graph for this function:

10.6.3.23 getObservedEvents()

```
std::vector< realtype > const & getObservedEvents ( ) const
```

get function that copies data from ExpData::mz to output

Returns

observed event data

Definition at line 209 of file edata.cpp.

10.6.3.24 getObservedEventsPtr()

```
const realtype * getObservedEventsPtr (
            int ie ) const
```

get function that returns a pointer to observed data at ieth occurence

Parameters

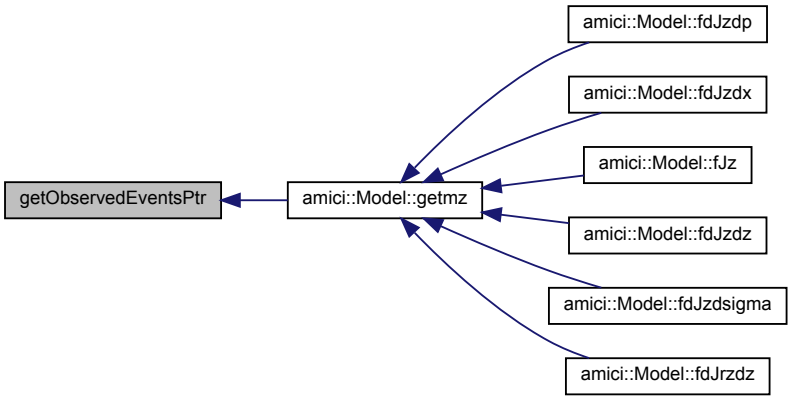
ie	event occurence

Returns

pointer to observed event data at ieth occurence

Definition at line 213 of file edata.cpp.

Here is the caller graph for this function:



10.6.3.25 setObservedEventsStdDev() [1/4]

```
void setObservedEventsStdDev (
            const std::vector< realtype > & observedEventsStdDev )
```

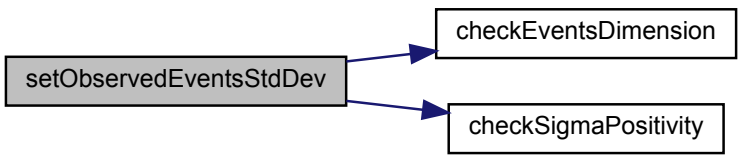
set function that copies data from input to ExpData::observedEventsStdDev

Parameters

observedEventsStdDev	standard deviation of observed event data

Definition at line 220 of file edata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.6.3.26 setObservedEventsStdDev() [2/4]

```
void setObservedEventsStdDev (
            const realtype stdDev )
```

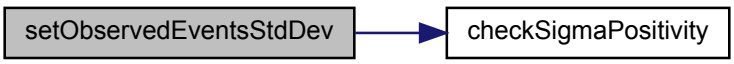
set function that sets all ExpData::observedDataStdDev to the input value

Parameters

stdDev	standard deviation (dimension: scalar)

Definition at line 230 of file edata.cpp.

Here is the call graph for this function:



10.6.3.27 setObservedEventsStdDev() [3/4]

```
void setObservedEventsStdDev (
            const std::vector< realtype > & observedEventsStdDev,
            int iz )
```

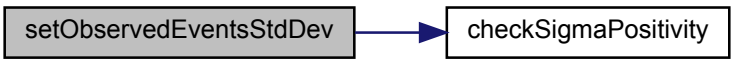
set function that copies standard deviation of observed data for specific observable

Parameters

observedEventsStdDev	standard deviation of observed data (dimension: nmaxevent)
iz	observed data index

Definition at line 235 of file edata.cpp.

Here is the call graph for this function:



10.6.3.28 setObservedEventsStdDev() [4/4]

```
void setObservedEventsStdDev (
            const realtype stdDev,
            int iz )
```

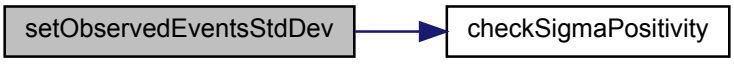
set function that sets all standard deviation of a specific observable to the input value

Parameters

stdDev	standard deviation (dimension: scalar)
iz	observed data index

Definition at line 244 of file edata.cpp.

Here is the call graph for this function:



10.6.3.29 isSetObservedEventsStdDev()

```
bool isSetObservedEventsStdDev (
            int ie,
            int iz ) const
```

get function that checks whether standard deviation of even data at specified indices has been set

Parameters

ie	event index
iz	event observable index

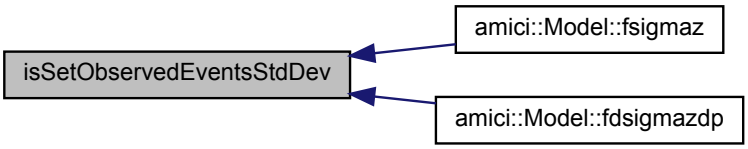
Returns

boolean specifying if standard deviation of event data was set

Definition at line 251 of file edata.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



10.6.3.30 getObservedEventsStdDev()

```
std::vector< realtype > const & getObservedEventsStdDev ( ) const
```

get function that copies data from ExpData::observedEventsStdDev to output

Returns

standard deviation of observed event data

Definition at line 258 of file edata.cpp.

10.6.3.31 getObservedEventsStdDevPtr()

```
const realtype * getObservedEventsStdDevPtr (
            int ie ) const
```

get function that returns a pointer to standard deviation of observed event data at ieth occurence

Parameters

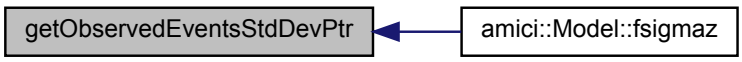
ie	event occurence

Returns

pointer to standard deviation of observed event data at ieth occurence

Definition at line 262 of file edata.cpp.

Here is the caller graph for this function:



10.6.3.32 checkDataDimension()

```
void checkDataDimension (
            std::vector< realtype > input,
            const char * fieldname ) const  [protected]
```

checker for dimensions of input observedData or observedDataStdDev

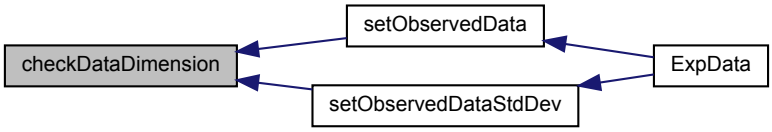
Parameters

input	vector input to be checked
fieldname	name of the input

Definition at line 269 of file edata.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



10.6.3.33 checkEventsDimension()

```
void checkEventsDimension (
            std::vector< realtype > input,
            const char * fieldname ) const  [protected]
```

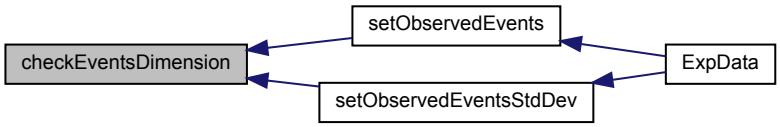
checker for dimensions of input observedEvents or observedEventsStdDev

Parameters

input	vector input to be checked
fieldname	name of the input

Definition at line 274 of file edata.cpp.

Here is the caller graph for this function:



10.6.3.34 checkSigmaPositivity() [1/2]

```
void checkSigmaPositivity (
            std::vector< realtype > sigmaVector,
            const char * vectorName ) const  [protected]
```

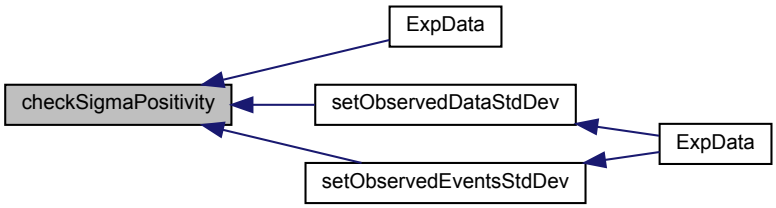
checks input vector of sigmas for not strictly positive values

Parameters

sigmaVector	vector input to be checked
vectorName	name of the input

Definition at line 279 of file edata.cpp.

Here is the caller graph for this function:



10.6.3.35 checkSigmaPositivity() [2/2]

```
void checkSigmaPositivity (
            realtype sigma,
            const char * sigmaName ) const  [protected]
```

checks input scalar sigma for not strictly positive value

Parameters

sigma	input to be checked
sigmaName	name of the input

Definition at line 284 of file edata.cpp.

10.6.4 Member Data Documentation

10.6.4.1 fixedParameters

```
std::vector<realtype> fixedParameters
```

condition-specific parameters of size Model::nk() or empty

Definition at line 327 of file edata.h.

10.6.4.2 fixedParametersPreequilibration

```
std::vector<realtype> fixedParametersPreequilibration
```

condition-specific parameters for pre-equilibration of size Model::nk() or empty. Overrides Solver::newton_preeq

Definition at line 330 of file edata.h.

10.6.4.3 fixedParametersPresimulation

```
std::vector<realtype> fixedParametersPresimulation
```

condition-specific parameters for pre-simulation of size Model::nk() or empty.

Definition at line 332 of file edata.h.

10.6.4.4 nytrue_

```
int nytrue_ [protected]
```

number of observables

Definition at line 375 of file edata.h.

10.6.4.5 nztrue_

```
int nztrue_ [protected]
```

number of event observables

Definition at line 378 of file edata.h.

10.6.4.6 nmaxevent_

```
int nmaxevent_ [protected]
```

maximal number of event occurences

Definition at line 381 of file edata.h.

10.6.4.7 ts

```
std::vector<realtype> ts [protected]
```

observation timepoints (dimension: nt)

Definition at line 384 of file edata.h.

10.6.4.8 observedData

```
std::vector<realtype> observedData [protected]
```

observed data (dimension: nt x nytrue, row-major)

Definition at line 387 of file edata.h.

10.6.4.9 observedDataStdDev

```
std::vector<realtype> observedDataStdDev [protected]
```

standard deviation of observed data (dimension: nt x nytrue, row-major)

Definition at line 389 of file edata.h.

10.6.4.10 observedEvents

```
std::vector<realtype> observedEvents [protected]
```

observed events (dimension: nmaxevents x nztrue, row-major)

Definition at line 392 of file edata.h.

10.6.4.11 observedEventsStdDev

```
std::vector<realtype> observedEventsStdDev [protected]
```

standard deviation of observed events/roots (dimension: nmaxevents x nztrue, row-major)

Definition at line 395 of file edata.h.

10.7 ForwardProblem Class Reference

The ForwardProblem class groups all functions for solving the backwards problem. Has only static members.

```
#include <forwardproblem.h>
```

Public Member Functions

- ForwardProblem (ReturnData *rdata, const ExpData *edata, Model *model, Solver *solver)
- void workForwardProblem ()
- realtype getTime () const
- AmiVectorArray const & getStateSensitivity () const
- AmiVectorArray const & getStatesAtDiscontinuities () const
- AmiVectorArray const & getRHSAtDiscontinuities () const
- AmiVectorArray const & getRHSBeforeDiscontinuities () const
- std::vector< int > const & getNumberOfRoots () const
- std::vector< realtype > const & getDiscontinuities () const
- std::vector< int > const & getRootIndexes () const
- std::vector< realtype > const & getDJydx () const
- std::vector< realtype > const & getDJzdx () const
- int getRootCounter () const
- AmiVector * getStatePointer ()
- AmiVector * getStateDerivativePointer ()
- AmiVectorArray * getStateSensitivityPointer ()
- AmiVectorArray * getStateDerivativeSensitivityPointer ()

Public Attributes

- Model * model
- ReturnData * rdata
- Solver * solver
- const ExpData * edata

10.7.1 Detailed Description

Definition at line 23 of file forwardproblem.h.

10.7.2 Constructor & Destructor Documentation

10.7.2.1 ForwardProblem()

```
ForwardProblem (
            ReturnData * rdata,
            const ExpData * edata,
            Model * model,
            Solver * solver )
```

Constructor

Parameters

rdata	pointer to ReturnData instance
edata	pointer to ExpData instance
model	pointer to Model instance
solver	pointer to Solver instance

Definition at line 42 of file forwardproblem.cpp.

10.7.3 Member Function Documentation

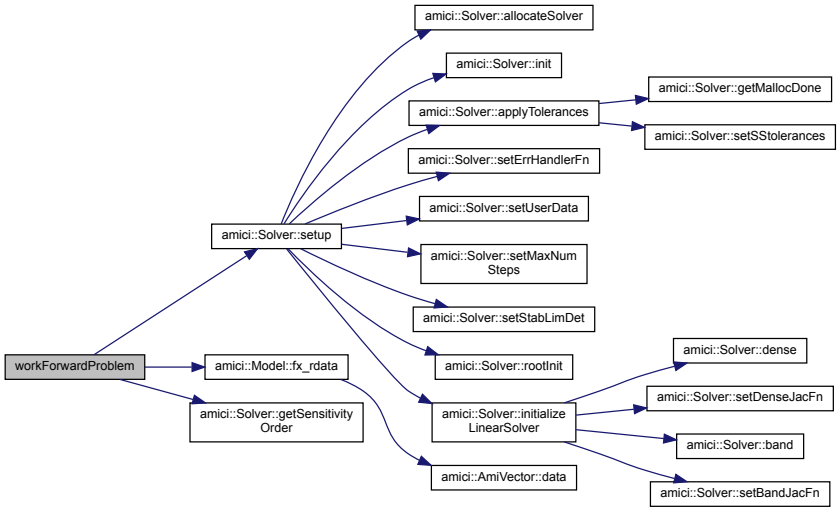
10.7.3.1 workForwardProblem()

```
void workForwardProblem ( )
```

workForwardProblem solves the forward problem. if forward sensitivities are enabled this will also compute sensitivies

Definition at line 81 of file forwardproblem.cpp.

Here is the call graph for this function:



10.7.3.2 getTime()

```
realtype getTime ( ) const
```

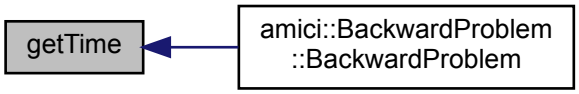
accessor for t

Returns

t

Definition at line 37 of file forwardproblem.h.

Here is the caller graph for this function:



10.7.3.3 getStateSensitivity()

```
AmiVectorArray const& getStateSensitivity ( ) const
```

accessor for sx

Returns

sx

Definition at line 44 of file forwardproblem.h.

10.7.3.4 getStatesAtDiscontinuities()

```
AmiVectorArray const& getStatesAtDiscontinuities ( ) const
```

accessor for x_disc

Returns

x_disc

Definition at line 51 of file forwardproblem.h.

10.7.3.5 getRHSAtDiscontinuities()

```
AmiVectorArray const& getRHSAtDiscontinuities ( ) const
```

accessor for xdot_disc

Returns

xdot_disc

Definition at line 58 of file forwardproblem.h.

10.7.3.6 getRHSBeforeDiscontinuities()

```
AmiVectorArray const& getRHSBeforeDiscontinuities ( ) const
```

accessor for xdot_old_disc

Returns

xdot_old_disc

Definition at line 65 of file forwardproblem.h.

10.7.3.7 getNumberOfRoots()

```
std::vector<int> const& getNumberOfRoots ( ) const
```

accessor for nroots

Returns

nroots

Definition at line 72 of file forwardproblem.h.

10.7.3.8 getDiscontinuities()

```
std::vector<realtype> const& getDiscontinuities ( ) const
```

accessor for discs

Returns

discs

Definition at line 79 of file forwardproblem.h.

10.7.3.9 getRootIndexes()

```
std::vector<int> const& getRootIndexes ( ) const
```

accessor for rootidx

Returns

rootidx

Definition at line 86 of file forwardproblem.h.

10.7.3.10 getDJydx()

```
std::vector<realtype> const& getDJydx ( ) const
```

accessor for dJydx

Returns

dJydx

Definition at line 93 of file forwardproblem.h.

10.7.3.11 getDJzdx()

```
std::vector<realtype> const& getDJzdx ( ) const
```

accessor for dJzdx

Returns

dJzdx

Definition at line 100 of file forwardproblem.h.

10.7.3.12 getRootCounter()

```
int getRootCounter ( ) const
```

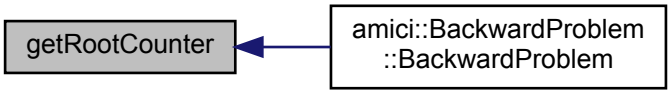
accessor for iroot

Returns

iroot

Definition at line 107 of file forwardproblem.h.

Here is the caller graph for this function:



10.7.3.13 getStatePointer()

```
AmiVector* getStatePointer ( )
```

accessor for pointer to x

Returns

&x

Definition at line 114 of file forwardproblem.h.

10.7.3.14 getStateDerivativePointer()

```
AmiVector* getStateDerivativePointer ( )
```

accessor for pointer to dx

Returns

&dx

Definition at line 121 of file forwardproblem.h.

10.7.3.15 getStateSensitivityPointer()

```
AmiVectorArray* getStateSensitivityPointer ( )
```

accessor for pointer to sx

Returns

&sx

Definition at line 128 of file forwardproblem.h.

10.7.3.16 getStateDerivativeSensitivityPointer()

```
AmiVectorArray* getStateDerivativeSensitivityPointer ( )
```

accessor for pointer to sdx

Returns

&sdx

Definition at line 135 of file forwardproblem.h.

10.7.4 Member Data Documentation

10.7.4.1 model

```
Model* model
```

pointer to model instance

Definition at line 140 of file forwardproblem.h.

10.7.4.2 rdata

```
ReturnData* rdata
```

pointer to return data instance

Definition at line 142 of file forwardproblem.h.

10.7.4.3 solver

```
Solver* solver
```

pointer to solver instance

Definition at line 144 of file forwardproblem.h.

10.7.4.4 edata

```
const ExpData* edata
```

pointer to experimental data instance

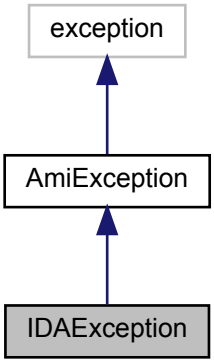
Definition at line 146 of file forwardproblem.h.

10.8 IDAException Class Reference

ida exception handler class

```
#include <exception.h>
```

Inheritance diagram for IDAException:



Public Member Functions

- IDAException (const int error_code, const char *function)

10.8.1 Detailed Description

Definition at line 129 of file exception.h.

10.8.2 Constructor & Destructor Documentation

10.8.2.1 IDAException()

```
IDAException (
            const int error_code,
            const char * function )
```

constructor

Parameters

error_code	error code returned by ida function
function	ida function name

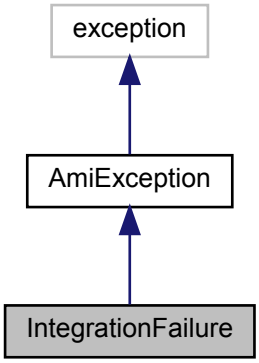
Definition at line 135 of file exception.h.

10.9 IntegrationFailure Class Reference

integration failure exception for the forward problem this exception should be thrown when an integration failure occured for this exception we can assume that we can recover from the exception and return a solution struct to the user

```
#include <exception.h>
```

Inheritance diagram for IntegrationFailure:



Public Member Functions

- IntegrationFailure (int code, realtype t)

Public Attributes

- int error_code
- realtype time

10.9.1 Detailed Description

Definition at line 144 of file exception.h.

10.9.2 Constructor & Destructor Documentation

10.9.2.1 IntegrationFailure()

```
IntegrationFailure (
            int code,
            realtype t )
```

constructor

Parameters

code	error code returned by cvode/ida
t	time of integration failure

Definition at line 154 of file exception.h.

10.9.3 Member Data Documentation

10.9.3.1 error_code

```
int error_code
```

error code returned by cvode/ida

Definition at line 147 of file exception.h.

10.9.3.2 time

```
realtype time
```

time of integration failure

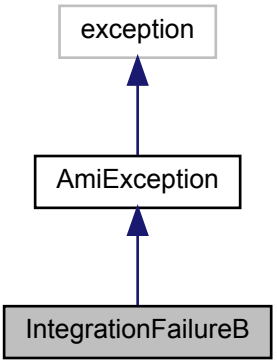
Definition at line 149 of file exception.h.

10.10 IntegrationFailureB Class Reference

integration failure exception for the backward problem this exception should be thrown when an integration failure occured for this exception we can assume that we can recover from the exception and return a solution struct to the user

```
#include <exception.h>
```

Inheritance diagram for IntegrationFailureB:



Public Member Functions

- IntegrationFailureB (int code, realtype t)

Public Attributes

- int error_code
- realtype time

10.10.1 Detailed Description

Definition at line 166 of file exception.h.

10.10.2 Constructor & Destructor Documentation

10.10.2.1 IntegrationFailureB()

```
IntegrationFailureB (
            int code,
            realtype t )
```

constructor

Parameters

code	error code returned by cvode/ida
t	time of integration failure

Definition at line 176 of file exception.h.

10.10.3 Member Data Documentation

10.10.3.1 error_code

```
int error_code
```

error code returned by cvode/ida

Definition at line 169 of file exception.h.

10.10.3.2 time

```
realtype time
```

time of integration failure

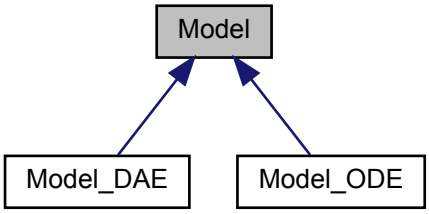
Definition at line 171 of file exception.h.

10.11 Model Class Reference

The Model class represents an AMICI ODE model. The model can compute various model related quantities based on symbolically generated code.

```
#include <model.h>
```

Inheritance diagram for Model:



Public Member Functions

- Model ()
- Model (const int nx_rdata, const int nxtrue_rdata, const int nx_solver, const int nxtrue_solver, const int ny, const int nytrue, const int nz, const int nztrue, const int ne, const int nJ, const int nw, const int ndwdx, const int ndwdp, const int nnz, const int ubw, const int lbw, amici::SecondOrderMode o2mode, const std::vector< amici::realtype > &p, std::vector< amici::realtype > k, const std::vector< int > &plist, std::vector< amici::realtype > idlist, std::vector< int > z2event)
- Model (Model const &other)
- virtual ~Model ()
- Model & operator= (Model const &other)=delete
- virtual Model * clone () const =0

  Clone this instance.
- virtual std::unique_ptr< Solver > getSolver ()=0
- virtual void froot (realtype t, AmiVector *x, AmiVector *dx, realtype *root)=0
- virtual void fxdot (realtype t, AmiVector *x, AmiVector *dx, AmiVector *xdot)=0
- virtual void fsxdot (realtype t, AmiVector *x, AmiVector *dx, int ip, AmiVector *sx, AmiVector *sdx, AmiVector *sxdot)=0
- virtual void fJ (realtype t, realtype cj, AmiVector *x, AmiVector *dx, AmiVector *xdot, DlsMat J)=0
- virtual void fJSparse (realtype t, realtype cj, AmiVector *x, AmiVector *dx, AmiVector *xdot, SlsMat J)=0
- virtual void fJDiag (realtype t, AmiVector *Jdiag, realtype cj, AmiVector *x, AmiVector *dx)=0
- virtual void fdxdotdp (realtype t, AmiVector *x, AmiVector *dx)=0
- virtual void fJv (realtype t, AmiVector *x, AmiVector *dx, AmiVector *xdot, AmiVector *v, AmiVector *nJv, realtype cj)=0
- void fx_rdata (AmiVector *x_rdata, const AmiVector *x_solver)
- void fsx_rdata (AmiVectorArray *sx_rdata, const AmiVectorArray *sx_solver)
- void fx0 (AmiVector *x)
- void fx0_fixedParameters (AmiVector *x)
- virtual void fdx0 (AmiVector *x0, AmiVector *dx0)
- void fsx0 (AmiVectorArray *sx, const AmiVector *x)
- void fsx0_fixedParameters (AmiVectorArray *sx, const AmiVector *x)
- virtual void fsdx0 ()
- void fstau (const realtype t, const int ie, const AmiVector *x, const AmiVectorArray *sx)
- void fy (const realtype t, const int it, const AmiVector *x, ReturnData *rdata)
- void fdydp (const realtype t, const AmiVector *x)
- void fdydx (const realtype t, const AmiVector *x)
- void fz (const int nroots, const int ie, const realtype t, const AmiVector *x, ReturnData *rdata)
- void fsz (const int nroots, const int ie, const realtype t, const AmiVector *x, const AmiVectorArray *sx, ReturnData *rdata)
- void frz (const int nroots, const int ie, const realtype t, const AmiVector *x, ReturnData *rdata)
- void fsrz (const int nroots, const int ie, const realtype t, const AmiVector *x, const AmiVectorArray *sx, ReturnData *rdata)
- void fdzdp (const realtype t, const int ie, const AmiVector *x)
- void fdzdx (const realtype t, const int ie, const AmiVector *x)
- void fdrzdp (const realtype t, const int ie, const AmiVector *x)
- void fdrzdx (const realtype t, const int ie, const AmiVector *x)
- void fdeltax (const int ie, const realtype t, const AmiVector *x, const AmiVector *xdot, const AmiVector *xdot_old)
- void fdeltasx (const int ie, const realtype t, const AmiVector *x, const AmiVectorArray *sx, const AmiVector *xdot, const AmiVector *xdot_old)
- void fdeltaxB (const int ie, const realtype t, const AmiVector *x, const AmiVector *xB, const AmiVector *xdot, const AmiVector *xdot_old)
- void fdeltaqB (const int ie, const realtype t, const AmiVector *x, const AmiVector *xB, const AmiVector *xdot, const AmiVector *xdot_old)
- void fsigmay (const int it, ReturnData *rdata, const ExpData *edata)

- void fdsigmaydp (const int it, ReturnData *rdata, const ExpData *edata)
- void fsigmaz (const realtype t, const int ie, const int *nroots, ReturnData *rdata, const ExpData *edata)
- void fdsigmazdp (const realtype t, const int ie, const int *nroots, ReturnData *rdata, const ExpData *edata)
- void fJy (const int it, ReturnData *rdata, const ExpData *edata)
- void fJz (const int nroots, ReturnData *rdata, const ExpData *edata)
- void fJrz (const int nroots, ReturnData *rdata, const ExpData *edata)
- void fdJydy (const int it, const ReturnData *rdata, const ExpData *edata)
- void fdJydsigma (const int it, const ReturnData *rdata, const ExpData *edata)
- void fdJzdz (const int nroots, const ReturnData *rdata, const ExpData *edata)
- void fdJzdsigma (const int nroots, const ReturnData *rdata, const ExpData *edata)
- void fdJrzdz (const int nroots, const ReturnData *rdata, const ExpData *edata)
- void fdJrzdsigma (const int nroots, const ReturnData *rdata, const ExpData *edata)
- void fsy (const int it, const AmiVectorArray *sx, ReturnData *rdata)
- void fsz_tf (const int *nroots, const int ie, ReturnData *rdata)
- void fsJy (const int it, const std::vector< realtype > &dJydx, const AmiVectorArray *sx, ReturnData *rdata)
- void fdJydp (const int it, ReturnData *rdata, const ExpData *edata)
- void fdJydx (std::vector< realtype > *dJydx, const int it, const ReturnData *rdata, const ExpData *edata)
- void fsJz (const int nroots, const std::vector< realtype > &dJzdx, const AmiVectorArray *sx, ReturnData *rdata)
- void fdJzdp (const int nroots, realtype t, const ExpData *edata, const ReturnData *rdata)
- void fdJzdx (std::vector< realtype > *dJzdx, const int nroots, realtype t, const ExpData *edata, const ReturnData *rdata)
- void initialize (AmiVector *x, AmiVector *dx)
- void initializeStates (AmiVector *x)
- void initHeaviside (AmiVector *x, AmiVector *dx)
- int nplist () const

  number of paramaeters wrt to which sensitivities are computed
- int np () const

  total number of model parameters
- int nk () const

  number of constants
- int ncl () const

  number of conservation laws
- const double * k () const

  fixed parameters
- int nMaxEvent () const

  Get nmaxevent.
- void setNMaxEvent (int nmaxevent)

  Set nmaxevent.
- int nt () const

  Get number of timepoints.
- std::vector< ParameterScaling > const & getParameterScale () const

  Get ParameterScale for each parameter.
- void setParameterScale (ParameterScaling pscale)

  Set ParameterScale for each parameter.
- void setParameterScale (const std::vector< ParameterScaling > &pscale)

  Set ParameterScale for each parameter.
- std::vector< realtype > const & getParameters () const

  Get the parameter vector.
- void setParameters (std::vector< realtype > const &p)

  Sets the parameter vector.
- std::vector< realtype > const & getUnscaledParameters () const

Gets parameters with transformation according to ParameterScale applied.

- std::vector< realtype > const & getFixedParameters () const

  Gets the fixedParameter member.
- void setFixedParameters (std::vector< realtype > const &k)

  Sets the fixedParameter member.
- realtype getFixedParameterById (std::string const &par_id) const

  Get value of fixed parameter with the specified Id.
- realtype getFixedParameterByName (std::string const &par_name) const

  Get value of fixed parameter with the specified name, if multiple parameters have the same name, the first parameter with matching name is returned.
- void setFixedParameterById (std::string const &par_id, realtype value)

  Set value of first fixed parameter with the specified id.
- int setFixedParametersByIdRegex (std::string const &par_id_regex, realtype value)

  Set values of all fixed parameters with the id matching the specified regex.
- void setFixedParameterByName (std::string const &par_name, realtype value)

  Set value of first fixed parameter with the specified name,.
- int setFixedParametersByNameRegex (std::string const &par_name_regex, realtype value)

  Set value of all fixed parameters with name matching the specified regex,.
- std::vector< realtype > const & getTimepoints () const

  Get the timepoint vector.
- void setTimepoints (std::vector< realtype > const &ts)

  Set the timepoint vector.
- std::vector< bool > const & getStateIsNonNegative () const

  gets flags indicating whether states should be treated as non-negative
- void setStateIsNonNegative (std::vector< bool > const &stateIsNonNegative)

  sets flags indicating whether states should be treated as non-negative
- double t (int idx) const

  Get timepoint for given index.
- std::vector< int > const & getParameterList () const

  Get the list of parameters for which sensitivities are computed.
- void setParameterList (std::vector< int > const &plist)

  Set the list of parameters for which sensitivities are computed.
- std::vector< realtype > const & getInitialStates () const

  Get the initial states.
- void setInitialStates (std::vector< realtype > const &x0)

  Set the initial states.
- std::vector< realtype > const & getInitialStateSensitivities () const

  Get the initial states sensitivities.
- void setInitialStateSensitivities (std::vector< realtype > const &sx0)

  Set the initial state sensitivities.
- double t0 () const

  get simulation start time
- void setT0 (double t0)

  set simulation start time
- int plist (int pos) const

  entry in parameter list
- void requireSensitivitiesForAllParameters ()

  Require computation of sensitivities for all parameters p [0..np[in natural order.
- void fw (const realtype t, const realtype *x)

  Recurring terms in xdot.
- void fdwdp (const realtype t, const realtype *x)

Recurring terms in xdot, parameter derivative.

- void fdwdx (const realtype t, const realtype ∗x)

  Recurring terms in xdot, state derivative.
- void fres (const int it, ReturnData ∗rdata, const ExpData ∗edata)
- void fchi2 (const int it, ReturnData ∗rdata)
- void fsres (const int it, ReturnData ∗rdata, const ExpData ∗edata)
- void fFIM (const int it, ReturnData ∗rdata)
- void updateHeaviside (const std::vector< int > &rootsfound)
- void updateHeavisideB (const int ∗rootsfound)
- realtype gett (const int it, const ReturnData ∗rdata) const
- int checkFinite (const int N, const realtype ∗array, const char ∗fun) const

  Check if the given array has only finite elements. If not try to give hints by which other fields this could be caused.
- virtual bool hasParameterNames () const

  Reports whether the model has parameter names set.
- virtual std::vector< std::string > getParameterNames () const

  Get names of the model parameters.
- virtual bool hasStateNames () const

  Reports whether the model has state names set.
- virtual std::vector< std::string > getStateNames () const

  Get names of the model states.
- virtual bool hasFixedParameterNames () const

  Reports whether the model has fixed parameter names set.
- virtual std::vector< std::string > getFixedParameterNames () const

  Get names of the fixed model parameters.
- virtual bool hasObservableNames () const

  Reports whether the model has observable names set.
- virtual std::vector< std::string > getObservableNames () const

  Get names of the observables.
- virtual bool hasParameterIds () const

  Reports whether the model has parameter ids set.
- virtual std::vector< std::string > getParameterIds () const

  Get ids of the model parameters.
- realtype getParameterById (std::string const &par_id) const

  Get value of first model parameter with the specified id.
- realtype getParameterByName (std::string const &par_name) const

  Get value of first model parameter with the specified name,.
- void setParameterById (std::string const &par_id, realtype value)

  Set value of first model parameter with the specified id.
- int setParametersByIdRegex (std::string const &par_id_regex, realtype value)

  Set all values of model parameters with ids matching the specified regex.
- void setParameterByName (std::string const &par_name, realtype value)

  Set value of first model parameter with the specified name.
- int setParametersByNameRegex (std::string const &par_name_regex, realtype value)

  Set all values of all model parameters with names matching the specified regex.
- virtual bool hasStateIds () const

  Reports whether the model has state ids set.
- virtual std::vector< std::string > getStateIds () const

  Get ids of the model states.
- virtual bool hasFixedParameterIds () const

  Reports whether the model has fixed parameter ids set.
- virtual std::vector< std::string > getFixedParameterIds () const

Get ids of the fixed model parameters.

- virtual bool hasObservableIds () const

  Reports whether the model has observable ids set.

- virtual std::vector< std::string > getObservableIds () const

  Get ids of the observables.

- void setSteadyStateSensitivityMode (const SteadyStateSensitivityMode mode)

  sets the mode how sensitivities are computed in the steadystate simulation

- SteadyStateSensitivityMode getSteadyStateSensitivityMode () const

  gets the mode how sensitivities are computed in the steadystate simulation

- void setReinitializeFixedParameterInitialStates (bool flag)

  set whether initial states depending on fixedParmeters are to be reinitialized after preequilibration and presimulation

- bool getReinitializeFixedParameterInitialStates () const

  get whether initial states depending on fixedParmeters are to be reinitialized after preequilibration and presimulation

Public Attributes

- const int nx_rdata
- const int nxtrue_rdata
- const int nx_solver
- const int nxtrue_solver
- const int ny
- const int nytrue
- const int nz
- const int nztrue
- const int ne
- const int nw
- const int ndwdx
- const int ndwdp
- const int nnz
- const int nJ
- const int ubw
- const int lbw
- const SecondOrderMode o2mode
- const std::vector< int > z2event
- const std::vector< realtype > idlist
- std::vector< realtype > sigmay
- std::vector< realtype > dsigmaydp
- std::vector< realtype > sigmaz
- std::vector< realtype > dsigmazdp
- std::vector< realtype > dJydp
- std::vector< realtype > dJzdp
- std::vector< realtype > deltax
- std::vector< realtype > deltasx
- std::vector< realtype > deltaxB
- std::vector< realtype > deltaqB
- std::vector< realtype > dxdotdp

Protected Member Functions

- void initializeVectors ()

  Set the nplist-dependent vectors to their proper sizes.
- virtual void fx_rdata (realtype ∗x_rdata, const realtype ∗x_solver, const realtype ∗tcl)
- virtual void fsx_rdata (realtype ∗sx_rdata, const realtype ∗sx_solver, const realtype ∗stcl, const int ip)
- virtual void fx_solver (realtype ∗x_solver, const realtype ∗x_rdata)
- virtual void fsx_solver (realtype ∗sx_solver, const realtype ∗sx_rdata)
- virtual void ftotal_cl (realtype ∗total_cl, const realtype ∗x_rdata)
- virtual void fstotal_cl (realtype ∗stotal_cl, const realtype ∗sx_rdata, const int ip)
- virtual void fx0 (realtype ∗x0, const realtype t, const realtype ∗p, const realtype ∗k)
- virtual void fx0_fixedParameters (realtype ∗x0, const realtype t, const realtype ∗p, const realtype ∗k)
- virtual void fsx0_fixedParameters (realtype ∗sx0, const realtype t, const realtype ∗x0, const realtype ∗p, const realtype ∗k, const int ip)
- virtual void fsx0 (realtype ∗sx0, const realtype t, const realtype ∗x0, const realtype ∗p, const realtype ∗k, const int ip)
- virtual void fstau (realtype ∗stau, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const realtype ∗sx, const int ip, const int ie)
- virtual void fy (realtype ∗y, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const realtype ∗w)
- virtual void fdydp (realtype ∗dydp, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const int ip, const realtype ∗w, const realtype ∗dwdp)
- virtual void fdydx (realtype ∗dydx, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const realtype ∗w, const realtype ∗dwdx)
- virtual void fz (realtype ∗z, const int ie, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h)
- virtual void fsz (realtype ∗sz, const int ie, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const realtype ∗sx, const int ip)
- virtual void frz (realtype ∗rz, const int ie, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h)
- virtual void fsrz (realtype ∗srz, const int ie, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const realtype ∗sx, const int ip)
- virtual void fdzdp (realtype ∗dzdp, const int ie, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const int ip)
- virtual void fdzdx (realtype ∗dzdx, const int ie, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h)
- virtual void fdrzdp (realtype ∗drzdp, const int ie, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const int ip)
- virtual void fdrzdx (realtype ∗drzdx, const int ie, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h)
- virtual void fdeltax (realtype ∗deltax, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const int ie, const realtype ∗xdot, const realtype ∗xdot_old)
- virtual void fdeltasx (realtype ∗deltasx, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const realtype ∗w, const int ip, const int ie, const realtype ∗xdot, const realtype ∗xdot_old, const realtype ∗sx, const realtype ∗stau)
- virtual void fdeltaxB (realtype ∗deltaxB, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const int ie, const realtype ∗xdot, const realtype ∗xdot_old, const realtype ∗xB)
- virtual void fdeltaqB (realtype ∗deltaqB, const realtype t, const realtype ∗x, const realtype ∗p, const realtype ∗k, const realtype ∗h, const int ip, const int ie, const realtype ∗xdot, const realtype ∗xdot_old, const realtype ∗xB)
- virtual void fsigmay (realtype ∗sigmay, const realtype t, const realtype ∗p, const realtype ∗k)
- virtual void fdsigmaydp (realtype ∗dsigmaydp, const realtype t, const realtype ∗p, const realtype ∗k, const int ip)
- virtual void fsigmaz (realtype ∗sigmaz, const realtype t, const realtype ∗p, const realtype ∗k)
- virtual void fdsigmazdp (realtype ∗dsigmazdp, const realtype t, const realtype ∗p, const realtype ∗k, const int ip)

- virtual void fJy (realtype *nllh, const int iy, const realtype *p, const realtype *k, const realtype *y, const realtype *sigmay, const realtype *my)
- virtual void fJz (realtype *nllh, const int iz, const realtype *p, const realtype *k, const realtype *z, const realtype *sigmaz, const realtype *mz)
- virtual void fJrz (realtype *nllh, const int iz, const realtype *p, const realtype *k, const realtype *z, const realtype *sigmaz)
- virtual void fdJydy (realtype *dJydy, const int iy, const realtype *p, const realtype *k, const realtype *y, const realtype *sigmay, const realtype *my)
- virtual void fdJydsigma (realtype *dJydsigma, const int iy, const realtype *p, const realtype *k, const realtype *y, const realtype *sigmay, const realtype *my)
- virtual void fdJzdz (realtype *dJzdz, const int iz, const realtype *p, const realtype *k, const realtype *z, const realtype *sigmaz, const realtype *mz)
- virtual void fdJzdsigma (realtype *dJzdsigma, const int iz, const realtype *p, const realtype *k, const realtype *z, const realtype *sigmaz, const realtype *mz)
- virtual void fdJrzdz (realtype *dJrzdz, const int iz, const realtype *p, const realtype *k, const realtype *rz, const realtype *sigmaz)
- virtual void fdJrzdsigma (realtype *dJrzdsigma, const int iz, const realtype *p, const realtype *k, const realtype *rz, const realtype *sigmaz)
- virtual void fw (realtype *w, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *tcl)
- virtual void fdwdp (realtype *dwdp, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *w, const realtype *tcl, const realtype *stcl)
- virtual void fdwdx (realtype *dwdx, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *w, const realtype *tcl)
- void getmy (const int it, const ExpData *edata)
- void getmz (const int nroots, const ExpData *edata)
- const realtype * gety (const int it, const ReturnData *rdata) const
- const realtype * getz (const int nroots, const ReturnData *rdata) const
- const realtype * getrz (const int nroots, const ReturnData *rdata) const
- const realtype * getsz (const int nroots, const int ip, const ReturnData *rdata) const
- const realtype * getsrz (const int nroots, const int ip, const ReturnData *rdata) const
- virtual bool isFixedParameterStateReinitializationAllowed () const
- N_Vector computeX_pos (N_Vector x)

  computes nonnegative state vector according to stateIsNonNegative if anyStateNonNegative is set to false, i.e., all entries in stateIsNonNegative are false, this function directly returns x, otherwise all entries of x are copied in to x_pos_tmp and negative values are replaced by 0 where applicable

Protected Attributes

- SlsMat J = nullptr
- std::vector< realtype > my
- std::vector< realtype > mz
- std::vector< realtype > dJydy
- std::vector< realtype > dJydsigma
- std::vector< realtype > dJzdz
- std::vector< realtype > dJzdsigma
- std::vector< realtype > dJrzdz
- std::vector< realtype > dJrzdsigma
- std::vector< realtype > dzdx
- std::vector< realtype > dzdp
- std::vector< realtype > drzdx
- std::vector< realtype > drzdp
- std::vector< realtype > dydp
- std::vector< realtype > dydx
- std::vector< realtype > w

- std::vector< realtype > dwdx
- std::vector< realtype > dwdp
- std::vector< realtype > M
- std::vector< realtype > stau
- std::vector< realtype > sx
- std::vector< realtype > x_rdata
- std::vector< realtype > sx_rdata
- std::vector< realtype > h
- std::vector< realtype > unscaledParameters
- std::vector< realtype > originalParameters
- std::vector< realtype > fixedParameters
- std::vector< realtype > total_cl
- std::vector< realtype > stotal_cl
- std::vector< int > plist_
- std::vector< double > x0data
- std::vector< realtype > sx0data
- std::vector< realtype > ts
- std::vector< bool > stateIsNonNegative
- bool anyStateNonNegative = false
- AmiVector x_pos_tmp
- int nmaxevent = 10
- std::vector< ParameterScaling > pscale
- double tstart = 0.0
- SteadyStateSensitivityMode steadyStateSensitivityMode = SteadyStateSensitivityMode::newtonOnly
- bool reinitializeFixedParameterInitialStates = false

Friends

- template<class Archive >
  void boost::serialization::serialize (Archive &ar, Model &r, const unsigned int version)

  Serialize Model (see boost::serialization::serialize)
- bool operator== (const Model &a, const Model &b)

  Check equality of data members.

10.11.1 Detailed Description

Definition at line 41 of file model.h.

10.11.2 Constructor & Destructor Documentation

10.11.2.1 Model() [1/3]

```
Model ( )
```

default constructor

Definition at line 44 of file model.h.

10.11.2.2 Model() [2/3]

```
Model (
            const int nx_rdata,
            const int nxtrue_rdata,
            const int nx_solver,
            const int nxtrue_solver,
            const int ny,
            const int nytrue,
            const int nz,
            const int nztrue,
            const int ne,
            const int nJ,
            const int nw,
            const int ndwdx,
            const int ndwdp,
            const int nnz,
            const int ubw,
            const int lbw,
            amici::SecondOrderMode o2mode,
            const std::vector< amici::realtype > & p,
            std::vector< amici::realtype > k,
            const std::vector< int > & plist,
            std::vector< amici::realtype > idlist,
            std::vector< int > z2event )
```

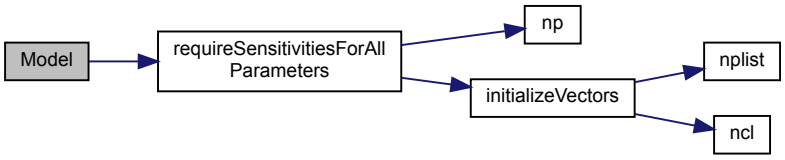
constructor with model dimensions

Parameters

nx_rdata	number of state variables
nxtrue_rdata	number of state variables of the non-augmented model
nx_solver	number of state variables with conservation laws applied
nxtrue_solver	number of state variables of the non-augmented model with conservation laws applied
ny	number of observables
nytrue	number of observables of the non-augmented model
nz	number of event observables
nztrue	number of event observables of the non-augmented model
ne	number of events
nJ	number of objective functions
nw	number of repeating elements
ndwdx	number of nonzero elements in the x derivative of the repeating elements
ndwdp	number of nonzero elements in the p derivative of the repeating elements
nnz	number of nonzero elements in Jacobian
ubw	upper matrix bandwidth in the Jacobian
lbw	lower matrix bandwidth in the Jacobian
o2mode	second order sensitivity mode
p	parameters
k	constants
plist	indexes wrt to which sensitivities are to be computed
idlist	indexes indicating algebraic components (DAE only)
z2event	mapping of event outputs to events

Definition at line 630 of file model.cpp.

Here is the call graph for this function:



10.11.2.3 Model() [3/3]

```
Model (
            Model const & other )
```

Copy constructor

Parameters

other	object to copy from

Returns

Definition at line 715 of file model.cpp.

10.11.2.4 ~Model()

```
~Model ( ) [virtual]
```

destructor

Definition at line 782 of file model.cpp.

10.11.3 Member Function Documentation

10.11.3.1 operator=()

```
Model& operator= (
            Model const & other ) [delete]
```

Copy assignment is disabled until const members are removed

Parameters

other	object to copy from

Returns

10.11.3.2 clone()

```
virtual Model* clone ( ) const  [pure virtual]
```

Returns

The clone

10.11.3.3 getSolver()

```
virtual std::unique_ptr<Solver> getSolver ( )  [pure virtual]
```

Retrieves the solver object

Returns

The Solver instance

Implemented in Model_DAE, and Model_ODE.

10.11.3.4 froot()

```
virtual void froot (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            realtype * root )  [pure virtual]
```

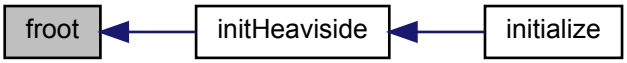
Root function

Parameters

t	time
x	state
dx	time derivative of state (DAE only)
root	array to which values of the root function will be written

Implemented in Model_DAE, and Model_ODE.

Here is the caller graph for this function:



10.11.3.5 fxdot()

```
virtual void fxdot (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot )  [pure virtual]
```

Residual function

Parameters

t	time
x	state
dx	time derivative of state (DAE only)
xdot	array to which values of the residual function will be written

Implemented in Model_ODE, and Model_DAE.

10.11.3.6 fsxdot()

```
virtual void fsxdot (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            int ip,
            AmiVector * sx,
            AmiVector * sdx,
            AmiVector * sxdot )  [pure virtual]
```

Sensitivity Residual function

Parameters

t	time
x	state

Parameters

dx	time derivative of state (DAE only)
ip	parameter index
sx	sensitivity state
sdx	time derivative of sensitivity state (DAE only)
sxdot	array to which values of the sensitivity residual function will be written

Implemented in Model_ODE, and Model_DAE.

10.11.3.7 fJ()

```
virtual void fJ (
            realtype t,
            realtype cj,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot,
            DlsMat J )  [pure virtual]
```

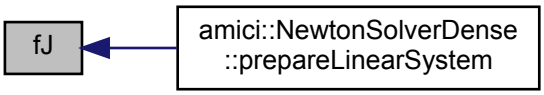
Dense Jacobian function

Parameters

t	time
cj	scaling factor (inverse of timestep, DAE only)
x	state
dx	time derivative of state (DAE only)
xdot	values of residual function (unused)
J	dense matrix to which values of the jacobian will be written

Implemented in Model_DAE, and Model_ODE.

Here is the caller graph for this function:



10.11.3.8 fJSparse()

```
virtual void fJSparse (
            realtype t,
            realtype cj,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot,
            SlsMat J )  [pure virtual]
```

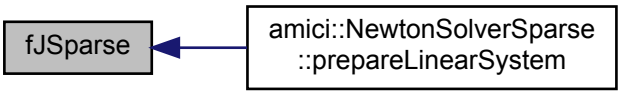
Sparse Jacobian function

Parameters

t	time
cj	scaling factor (inverse of timestep, DAE only)
x	state
dx	time derivative of state (DAE only)
xdot	values of residual function (unused)
J	sparse matrix to which values of the Jacobian will be written

Implemented in Model_DAE, and Model_ODE.

Here is the caller graph for this function:



10.11.3.9 fJDiag()

```
virtual void fJDiag (
            realtype t,
            AmiVector * Jdiag,
            realtype cj,
            AmiVector * x,
            AmiVector * dx )  [pure virtual]
```

Diagonal Jacobian function

Parameters

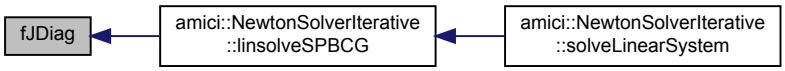
t	time
Jdiag	array to which the diagonal of the Jacobian will be written
cj	scaling factor (inverse of timestep, DAE only)
x	state
dx	time derivative of state (DAE only)

Returns

flag indicating successful evaluation

Implemented in Model_ODE, and Model_DAE.

Here is the caller graph for this function:



10.11.3.10 fdxdotdp()

```
virtual void fdxdotdp (
            realtype t,
            AmiVector * x,
            AmiVector * dx )  [pure virtual]
```

parameter derivative of residual function

Parameters

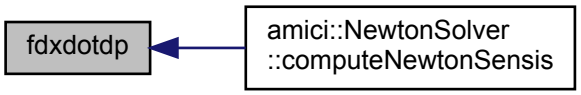
t	time
x	state
dx	time derivative of state (DAE only)

Returns

flag indicating successful evaluation

Implemented in Model_ODE, and Model_DAE.

Here is the caller graph for this function:



10.11.3.11 fJv()

```
virtual void fJv (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot,
            AmiVector * v,
            AmiVector * nJv,
            realtype cj )  [pure virtual]
```

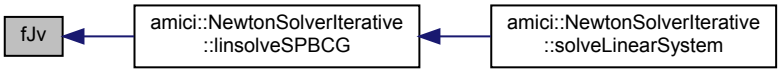
Jacobian multiply function

Parameters

t	time
x	state
dx	time derivative of state (DAE only)
xdot	values of residual function (unused)
v	multiplication vector (unused)
nJv	array to which result of multiplication will be written
cj	scaling factor (inverse of timestep, DAE only)

Implemented in Model_ODE, and Model_DAE.

Here is the caller graph for this function:



10.11.3.12 fx_rdata() [1/2]

```
void fx_rdata (
            AmiVector * x_rdata,
            const AmiVector * x_solver )
```

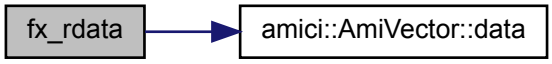
Expands conservation law for states

Parameters

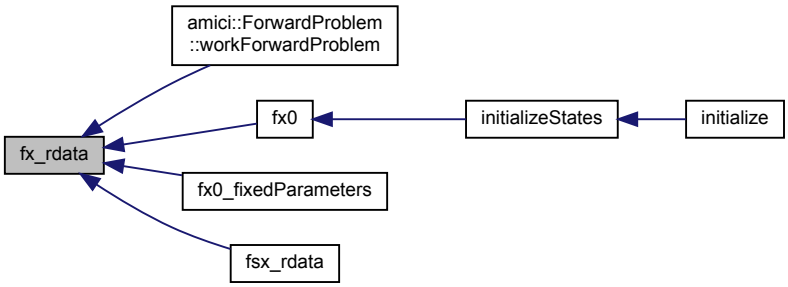
x_rdata	pointer to state variables with conservation laws expanded (stored in rdata)
x_solver	pointer to state variables with conservation laws applied (solver returns this)

Definition at line 804 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.13 fsx_rdata() [1/2]

```
void fsx_rdata (
            AmiVectorArray * sx_rdata,
            const AmiVectorArray * sx_solver )
```

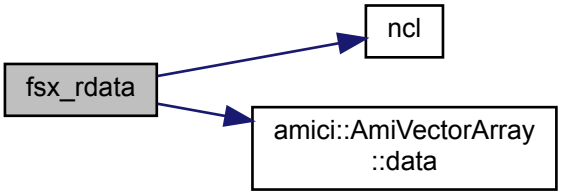
Expands conservation law for state sensitivities

Parameters

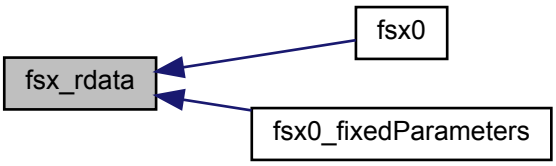
sx_rdata	pointer to state variable sensitivities with conservation laws expanded (stored in rdata)
sx_solver	pointer to state variable sensitivities with conservation laws applied (solver returns this)

Definition at line 835 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.14 fx0() [1/2]

```
void fx0 (
            AmiVector * x )
```

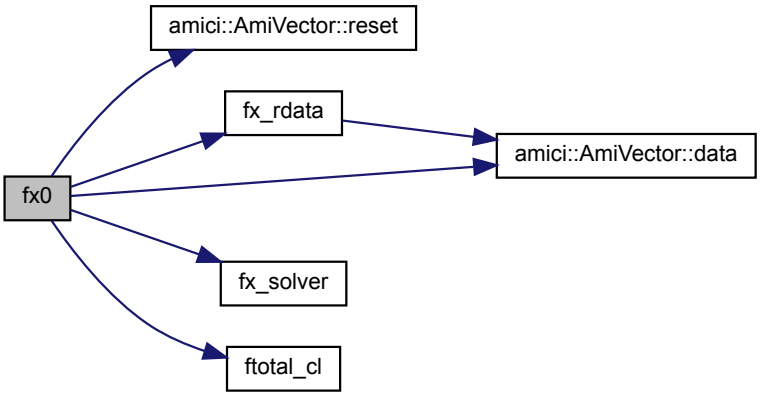
Initial states

Parameters

x	pointer to state variables

Definition at line 808 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.11.3.15 fx0_fixedParameters() [1/2]

```
void fx0_fixedParameters (
            AmiVector * x )
```

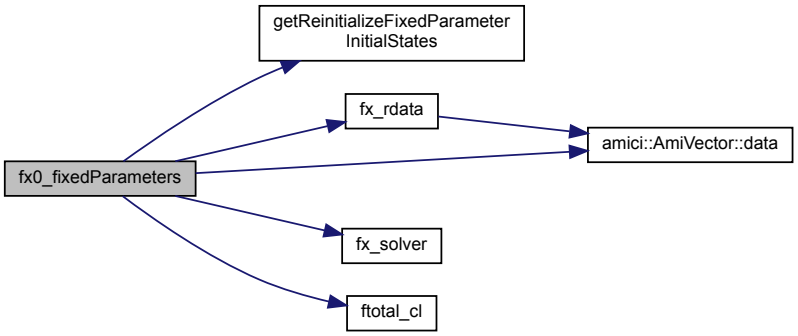
Sets only those initial states that are specified via fixedParmeters

Parameters

x	pointer to state variables

Definition at line 818 of file model.cpp.

Here is the call graph for this function:



10.11.3.16 fdx0()

```
void fdx0 (
            AmiVector * x0,
            AmiVector * dx0 )  [virtual]
```

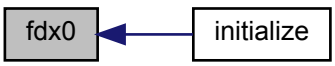
Initial value for time derivative of states (only necessary for DAEs)

Parameters

x0	Vector with the initial states
dx0	Vector to which the initial derivative states will be written (only DAE)

Definition at line 833 of file model.cpp.

Here is the caller graph for this function:



10.11.3.17 fsx0() [1/2]

```
void fsx0 (
            AmiVectorArray * sx,
            const AmiVector * x )
```

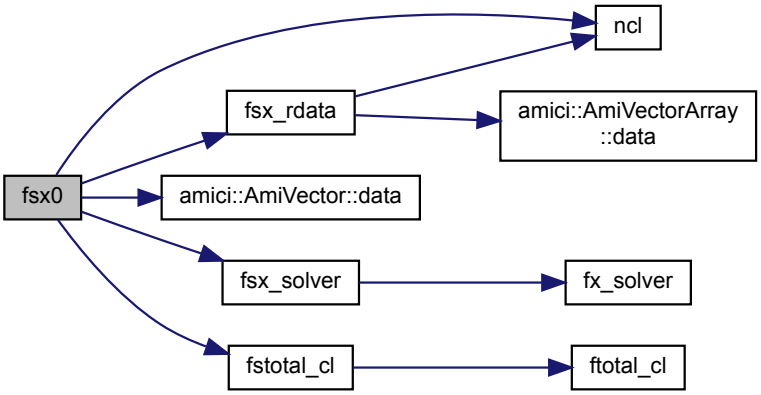
Initial value for initial state sensitivities

Parameters

sx	pointer to state sensitivity variables
x	pointer to state variables

Definition at line 844 of file model.cpp.

Here is the call graph for this function:



10.11.3.18 fsx0_fixedParameters() [1/2]

```
void fsx0_fixedParameters (
            AmiVectorArray * sx,
            const AmiVector * x )
```

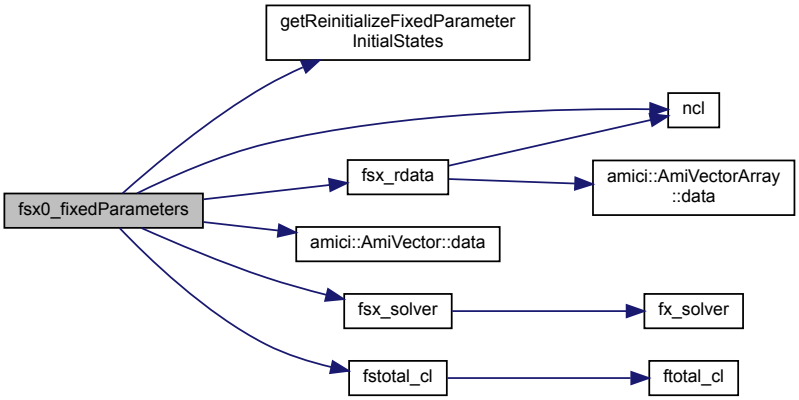
Sets only those initial states sensitivities that are affected from fx0 fixedParmeters

Parameters

sx	pointer to state sensitivity variables
x	pointer to state variables

Definition at line 858 of file model.cpp.

Here is the call graph for this function:



10.11.3.19 fsdx0()

```
void fsdx0 ( ) [virtual]
```

Sensitivity of derivative initial states sensitivities sdx0 (only necessary for DAEs)

Definition at line 874 of file model.cpp.

10.11.3.20 fstau() [1/2]

```
void fstau (
            const realtype t,
            const int ie,
            const AmiVector * x,
            const AmiVectorArray * sx )
```

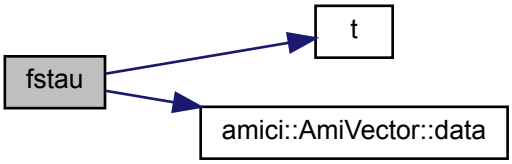
Sensitivity of event timepoint, total derivative

Parameters

t	current timepoint
ie	event index
x	pointer to state variables
sx	pointer to state sensitivity variables

Definition at line 876 of file model.cpp.

Here is the call graph for this function:



10.11.3.21 fy() [1/2]

```
void fy (
            const realtype t,
            const int it,
            const AmiVector * x,
            ReturnData * rdata )
```

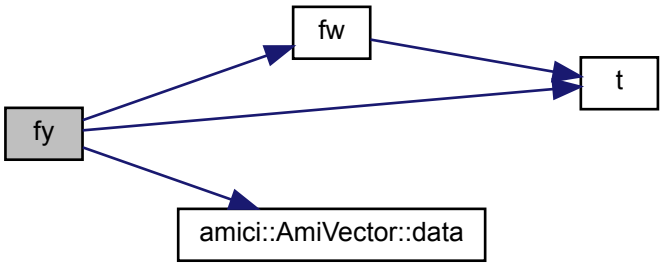
Observables / measurements

Parameters

t	current timepoint
it	timepoint index
x	current state
rdata	pointer to return data instance

Definition at line 883 of file model.cpp.

Here is the call graph for this function:



10.11.3.22 fdydp() [1/2]

```
void fdydp (
            const realtype t,
            const AmiVector * x )
```

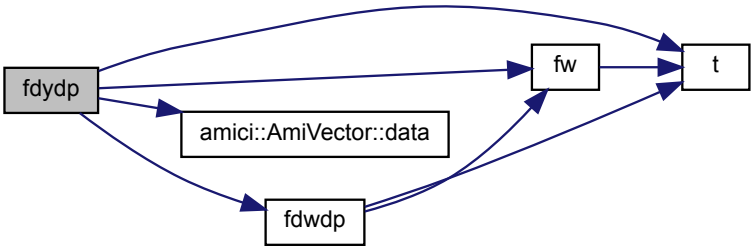
partial derivative of observables y w.r.t. model parameters p

Parameters

t	current timepoint
x	current state

Definition at line 890 of file model.cpp.

Here is the call graph for this function:



10.11.3.23 fdydx() [1/2]

```
void fdydx (
            const realtype t,
            const AmiVector * x )
```

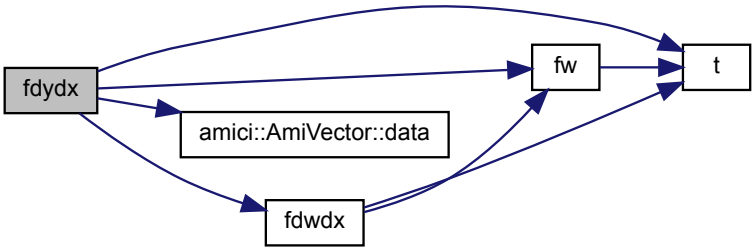
partial derivative of observables y w.r.t. state variables x

Parameters

t	current timepoint
x	current state

Definition at line 911 of file model.cpp.

Here is the call graph for this function:



10.11.3.24 fz() [1/2]

```
void fz (
            const int nroots,
            const int ie,
            const realtype t,
            const AmiVector * x,
            ReturnData * rdata )
```

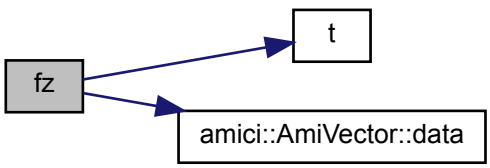
Event-resolved output

Parameters

nroots	number of events for event index
ie	event index
t	current timepoint
x	current state
rdata	pointer to return data instance

Definition at line 921 of file model.cpp.

Here is the call graph for this function:



10.11.3.25 fsz() [1/2]

```
void fsz (
            const int nroots,
            const int ie,
            const realtype t,
            const AmiVector * x,
            const AmiVectorArray * sx,
            ReturnData * rdata )
```

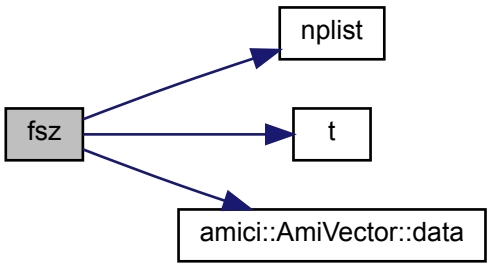
Sensitivity of z, total derivative

Parameters

nroots	number of events for event index
ie	event index
t	current timepoint
x	current state
sx	current state sensitivities
rdata	pointer to return data instance

Definition at line 925 of file model.cpp.

Here is the call graph for this function:



10.11.3.26 frz() [1/2]

```
void frz (
            const int nroots,
            const int ie,
            const realtype t,
            const AmiVector * x,
            ReturnData * rdata )
```

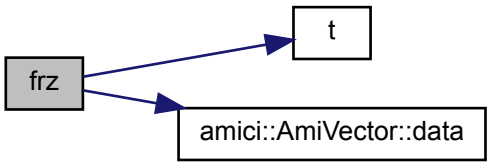
Event root function of events (equal to froot but does not include non-output events)

Parameters

nroots	number of events for event index
ie	event index
t	current timepoint
x	current state
rdata	pointer to return data instance

Definition at line 931 of file model.cpp.

Here is the call graph for this function:



10.11.3.27 fsrz() [1/2]

```
void fsrz (
            const int nroots,
            const int ie,
            const realtype t,
            const AmiVector * x,
            const AmiVectorArray * sx,
            ReturnData * rdata )
```

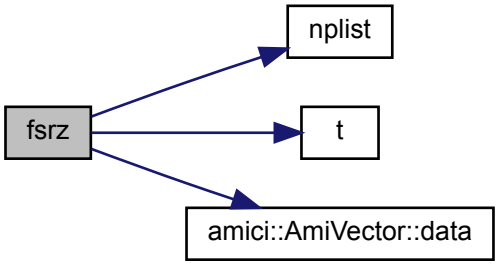
Sensitivity of rz, total derivative

Parameters

nroots	number of events for event index
ie	event index
t	current timepoint
x	current state
sx	current state sensitivities
rdata	pointer to return data instance

Definition at line 935 of file model.cpp.

Here is the call graph for this function:



10.11.3.28 fdzdp() [1/2]

```
void fdzdp (
            const realtype t,
            const int ie,
            const AmiVector * x )
```

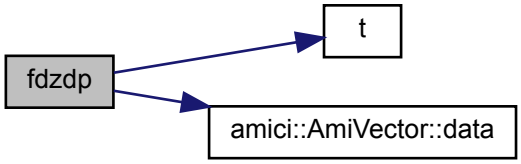
partial derivative of event-resolved output z w.r.t. to model parameters p

Parameters

ie	event index
t	current timepoint
x	current state

Definition at line 941 of file model.cpp.

Here is the call graph for this function:



10.11.3.29 fdzdx() [1/2]

```
void fdzdx (
            const realtype t,
            const int ie,
            const AmiVector * x )
```

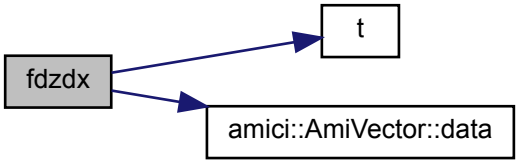
partial derivative of event-resolved output z w.r.t. to model states x

Parameters

ie	event index
t	current timepoint
x	current state

Definition at line 948 of file model.cpp.

Here is the call graph for this function:



10.11.3.30 fdrzdp() [1/2]

```
void fdrzdp (
            const realtype t,
            const int ie,
            const AmiVector * x )
```

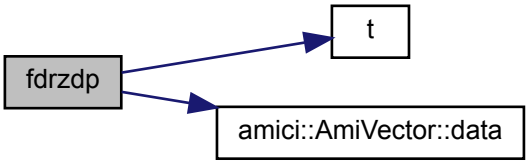
Sensitivity of event-resolved root output w.r.t. to model parameters p

Parameters

ie	event index
t	current timepoint
x	current state

Definition at line 953 of file model.cpp.

Here is the call graph for this function:



10.11.3.31 fdrzdx() [1/2]

```
void fdrzdx (
            const realtype t,
            const int ie,
            const AmiVector * x )
```

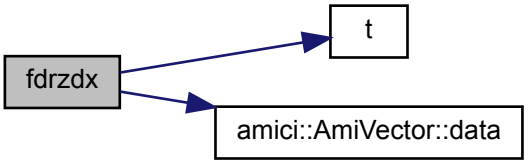
Sensitivity of event-resolved measurements rz w.r.t. to model states x

Parameters

ie	event index
t	current timepoint
x	current state

Definition at line 961 of file model.cpp.

Here is the call graph for this function:



10.11.3.32 fdeltax() [1/2]

```
void fdeltax (
            const int ie,
            const realtype t,
            const AmiVector * x,
            const AmiVector * xdot,
            const AmiVector * xdot_old )
```

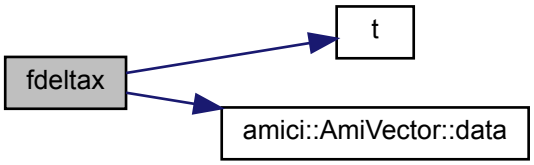
State update functions for events

Parameters

ie	event index
t	current timepoint
x	current state
xdot	current residual function values
xdot_old	value of residual function before event

Definition at line 966 of file model.cpp.

Here is the call graph for this function:



10.11.3.33 fdeltasx() [1/2]

```
void fdeltasx (
            const int ie,
            const realtype t,
            const AmiVector * x,
            const AmiVectorArray * sx,
            const AmiVector * xdot,
            const AmiVector * xdot_old )
```

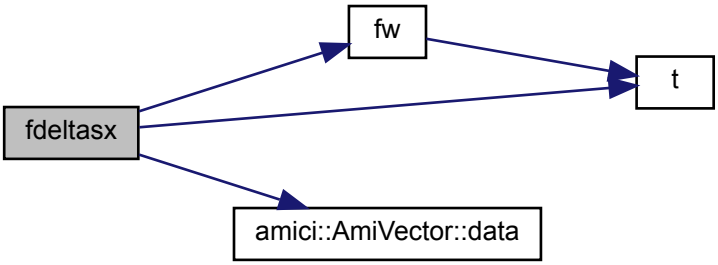
Sensitivity update functions for events, total derivative

Parameters

ie	event index
t	current timepoint
x	current state
sx	current state sensitivity
xdot	current residual function values
xdot_old	value of residual function before event

Definition at line 972 of file model.cpp.

Here is the call graph for this function:



10.11.3.34 fdeltaxB() [1/2]

```
void fdeltaxB (
            const int ie,
            const realtype t,
            const AmiVector * x,
            const AmiVector * xB,
            const AmiVector * xdot,
            const AmiVector * xdot_old )
```

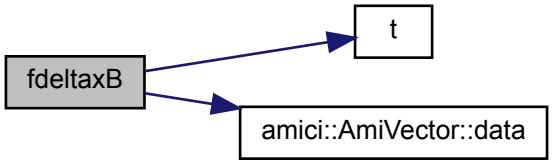
Adjoint state update functions for events

Parameters

ie	event index
t	current timepoint
x	current state
xB	current adjoint state
xdot	current residual function values
xdot_old	value of residual function before event

Definition at line 981 of file model.cpp.

Here is the call graph for this function:



10.11.3.35 fdeltaqB() [1/2]

```
void fdeltaqB (
            const int ie,
            const realtype t,
            const AmiVector * x,
            const AmiVector * xB,
            const AmiVector * xdot,
            const AmiVector * xdot_old )
```

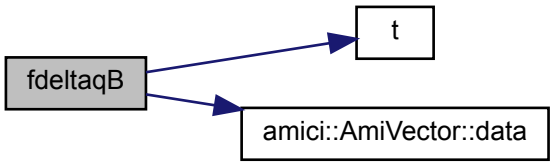
Quadrature state update functions for events

Parameters

ie	event index
t	current timepoint
x	current state
xB	current adjoint state
xdot	current residual function values
xdot_old	value of residual function before event

Definition at line 987 of file model.cpp.

Here is the call graph for this function:



10.11.3.36 fsigmay() [1/2]

```
void fsigmay (
            const int it,
            ReturnData * rdata,
            const ExpData * edata )
```

Standard deviation of measurements

Parameters

it	timepoint index
edata	pointer to experimental data instance
rdata	pointer to return data instance

Definition at line 995 of file model.cpp.

Here is the call graph for this function:

10.11.3.37 fdsigmaydp() [1/2]

```
void fdsigmaydp (
            const int it,
            ReturnData * rdata,
            const ExpData * edata )
```

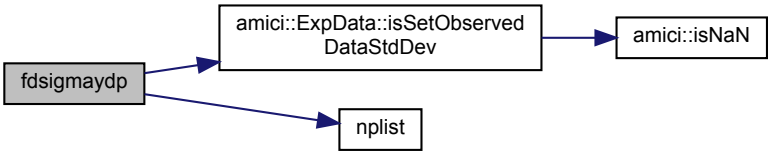
partial derivative of standard deviation of measurements w.r.t. model

Parameters

it	timepoint index
rdata	pointer to return data instance
edata	pointer to ExpData data instance holding sigma values

Definition at line 1014 of file model.cpp.

Here is the call graph for this function:



10.11.3.38 fsigmaz() [1/2]

```
void fsigmaz (
            const realtype t,
            const int ie,
            const int * nroots,
            ReturnData * rdata,
            const ExpData * edata )
```

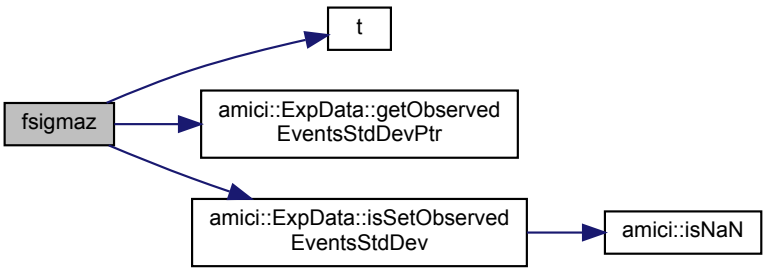
Standard deviation of events

Parameters

t	current timepoint
ie	event index
nroots	array with event numbers
edata	pointer to experimental data instance
rdata	pointer to return data instance

Definition at line 1043 of file model.cpp.

Here is the call graph for this function:



10.11.3.39 fdsigmazdp() [1/2]

```
void fdsigmazdp (
            const realtype t,
            const int ie,
            const int * nroots,
            ReturnData * rdata,
            const ExpData * edata )
```

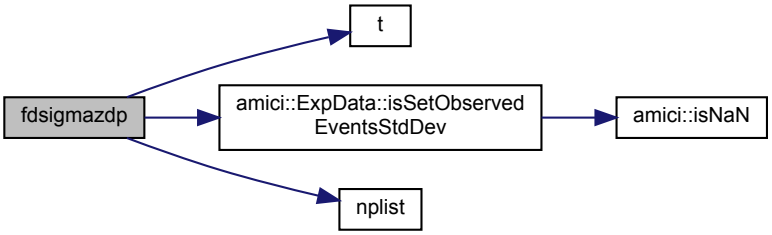
Sensitivity of standard deviation of events measurements w.r.t. model parameters p

Parameters

t	current timepoint
ie	event index
nroots	array with event numbers
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1061 of file model.cpp.

Here is the call graph for this function:



10.11.3.40 fJy() [1/2]

```
void fJy (
            const int it,
            ReturnData * rdata,
            const ExpData * edata )
```

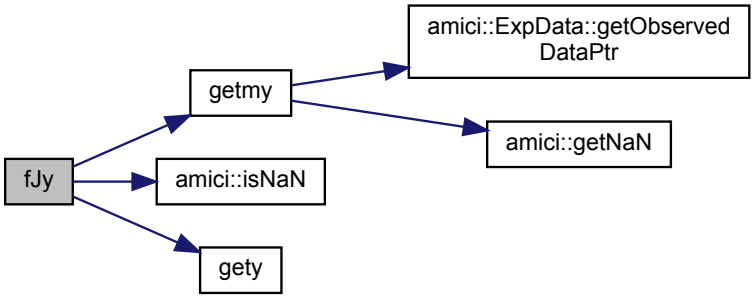
negative log-likelihood of measurements y

Parameters

it	timepoint index
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1086 of file model.cpp.

Here is the call graph for this function:



10.11.3.41 fJz() [1/2]

```
void fJz (
            const int nroots,
            ReturnData * rdata,
            const ExpData * edata )
```

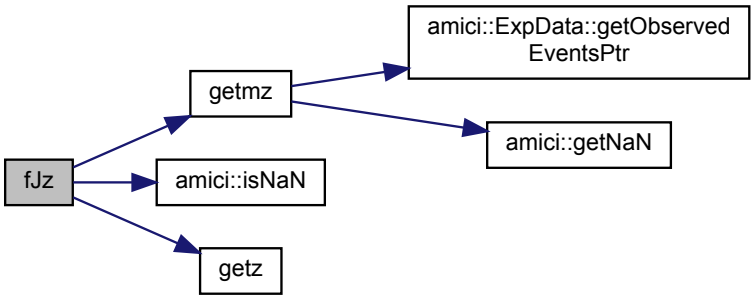
negative log-likelihood of event-resolved measurements z

Parameters

nroots	event index
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1098 of file model.cpp.

Here is the call graph for this function:



10.11.3.42 fJrz() [1/2]

```
void fJrz (
            const int nroots,
            ReturnData * rdata,
            const ExpData * edata )
```

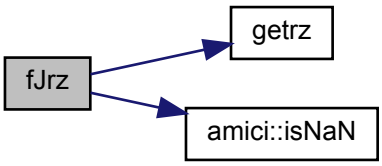
regularization of negative log-likelihood with roots of event-resolved measurements rz

Parameters

nroots	event index
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1110 of file model.cpp.

Here is the call graph for this function:



10.11.3.43 fdJydy() [1/2]

```
void fdJydy (
            const int it,
            const ReturnData * rdata,
            const ExpData * edata )
```

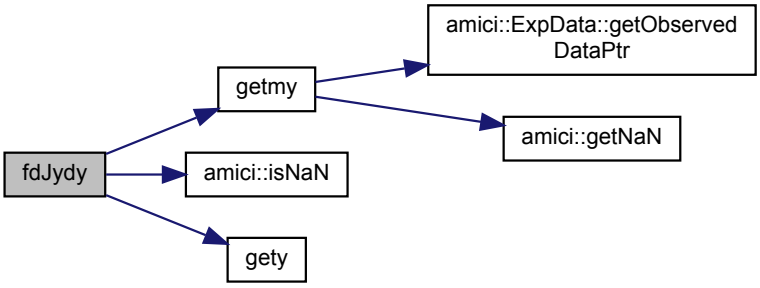
partial derivative of time-resolved measurement negative log-likelihood Jy

Parameters

it	timepoint index
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1122 of file model.cpp.

Here is the call graph for this function:



10.11.3.44 fdJydsigma() [1/2]

```
void fdJydsigma (
            const int it,
            const ReturnData * rdata,
            const ExpData * edata )
```

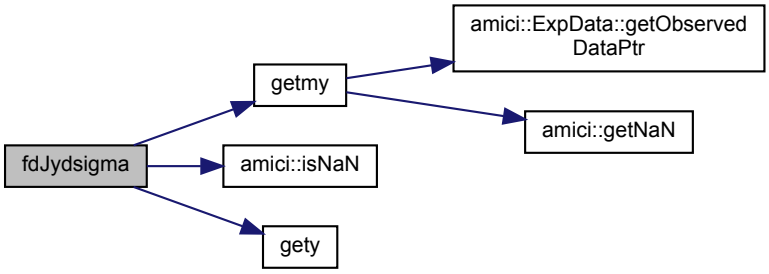
Sensitivity of time-resolved measurement negative log-likelihood Jy w.r.t. standard deviation sigma

Parameters

it	timepoint index
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1142 of file model.cpp.

Here is the call graph for this function:



10.11.3.45 fdJzdz() [1/2]

```
void fdJzdz (
            const int nroots,
            const ReturnData * rdata,
            const ExpData * edata )
```

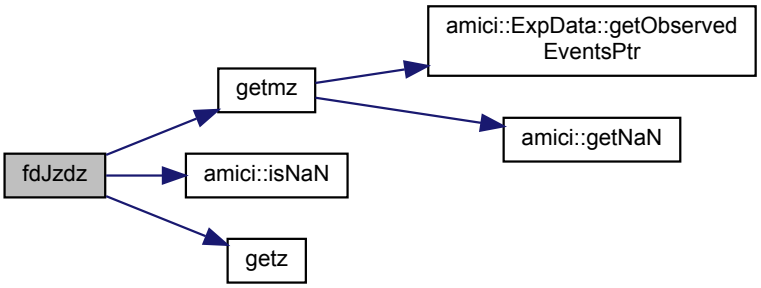
partial derivative of event measurement negative log-likelihood Jz

Parameters

nroots	event index
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1162 of file model.cpp.

Here is the call graph for this function:



10.11.3.46 fdJzdsigma() [1/2]

```
void fdJzdsigma (
            const int nroots,
            const ReturnData * rdata,
            const ExpData * edata )
```

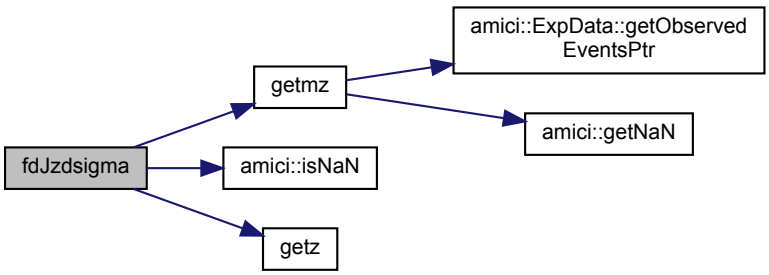
Sensitivity of event measurement negative log-likelihood Jz w.r.t. standard deviation sigmaz

Parameters

nroots	event index
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1173 of file model.cpp.

Here is the call graph for this function:



10.11.3.47 fdJrzdz() [1/2]

```
void fdJrzdz (
            const int nroots,
            const ReturnData * rdata,
            const ExpData * edata )
```

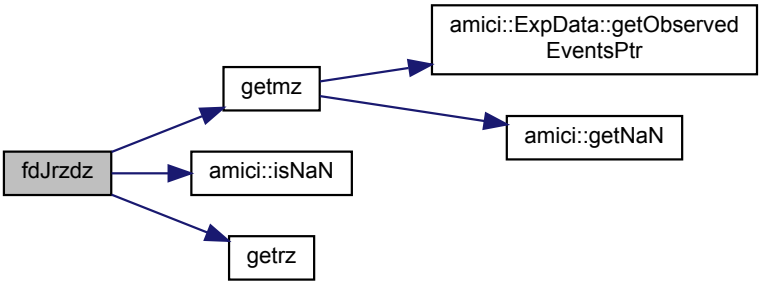
partial derivative of event measurement negative log-likelihood Jz

Parameters

nroots	event index
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1184 of file model.cpp.

Here is the call graph for this function:



10.11.3.48 fdJrzdsigma() [1/2]

```
void fdJrzdsigma (
            const int nroots,
            const ReturnData * rdata,
            const ExpData * edata )
```

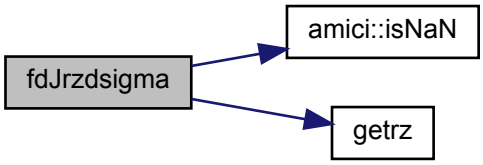
Sensitivity of event measurement negative log-likelihood Jz w.r.t. standard deviation sigmaz

Parameters

nroots	event index
rdata	pointer to return data instance
edata	pointer to experimental data instance

Definition at line 1195 of file model.cpp.

Here is the call graph for this function:



10.11.3.49 fsy()

```
void fsy (
            const int it,
            const AmiVectorArray * sx,
            ReturnData * rdata )
```

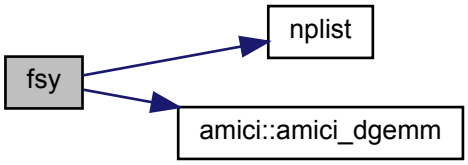
Sensitivity of measurements y, total derivative sy = dydx ∗ sx + dydp

Parameters

it	timepoint index
sx	pointer to state sensitivities
rdata	pointer to return data instance

Definition at line 13 of file model.cpp.

Here is the call graph for this function:



10.11.3.50 fsz_tf()

```
void fsz_tf (
            const int * nroots,
            const int ie,
            ReturnData * rdata )
```

Sensitivity of z at final timepoint (ignores sensitivity of timepoint), total derivative

Parameters

nroots	number of events for event index
ie	event index
rdata	pointer to return data instance

Definition at line 31 of file model.cpp.

Here is the call graph for this function:

10.11.3.51 fsJy()

```
void fsJy (
            const int it,
            const std::vector< realtype > & dJydx,
            const AmiVectorArray * sx,
            ReturnData * rdata )
```

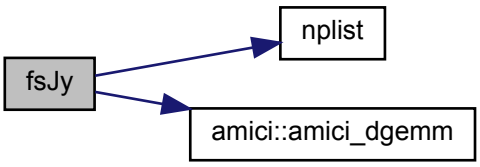
Sensitivity of time-resolved measurement negative log-likelihood Jy, total derivative

Parameters

it	timepoint index
sx	pointer to state sensitivities
dJydx	vector with values of state derivative of Jy
rdata	pointer to return data instance

Definition at line 38 of file model.cpp.

Here is the call graph for this function:



10.11.3.52 fdJydp()

```
void fdJydp (
            const int it,
            ReturnData * rdata,
            const ExpData * edata )
```

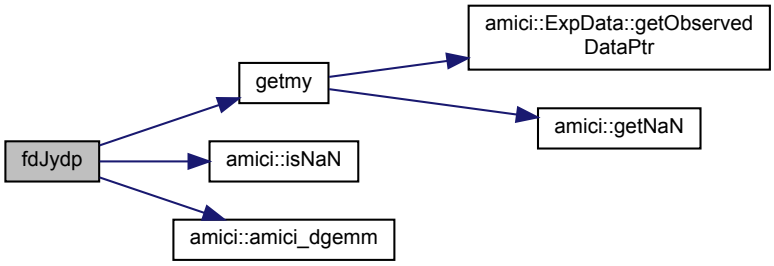
Compute sensitivity of time-resolved measurement negative log-likelihood Jy w.r.t. parameters for the given time-point. Add result to respective fields in rdata.

Parameters

it	timepoint index
edata	pointer to experimental data instance
rdata	pointer to return data instance

Definition at line 68 of file model.cpp.

Here is the call graph for this function:



10.11.3.53 fdJydx()

```
void fdJydx (
            std::vector< realtype > * dJydx,
            const int it,
            const ReturnData * rdata,
            const ExpData * edata )
```

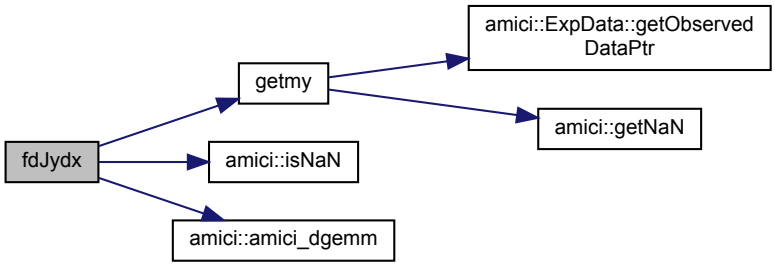
Sensitivity of time-resolved measurement negative log-likelihood Jy w.r.t. state variables

Parameters

dJydx	pointer to vector with values of state derivative of Jy
it	timepoint index
edata	pointer to experimental data instance
rdata	pointer to return data instance

Definition at line 115 of file model.cpp.

Here is the call graph for this function:



10.11.3.54 fsJz()

```
void fsJz (
            const int nroots,
            const std::vector< realtype > & dJzdx,
            const AmiVectorArray * sx,
            ReturnData * rdata )
```

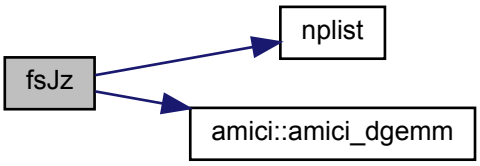
Sensitivity of event-resolved measurement negative log-likelihood Jz, total derivative

Parameters

nroots	event index
dJzdx	vector with values of state derivative of Jz
sx	pointer to state sensitivities
rdata	pointer to return data instance

Definition at line 134 of file model.cpp.

Here is the call graph for this function:



10.11.3.55 fdJzdp()

```
void fdJzdp (
            const int nroots,
            realtype t,
            const ExpData * edata,
            const ReturnData * rdata )
```

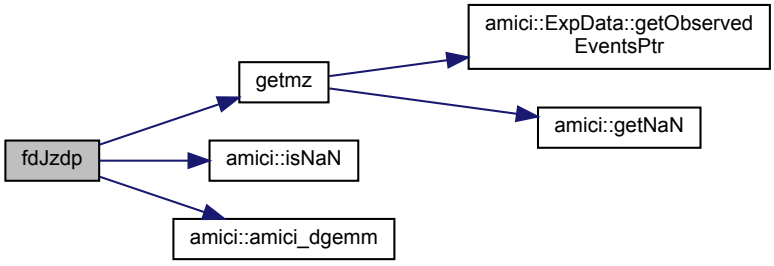
Sensitivity of event-resolved measurement negative log-likelihood Jz w.r.t. parameters

Parameters

nroots	event index
t	current timepoint
edata	pointer to experimental data instance
rdata	pointer to return data instance

Definition at line 164 of file model.cpp.

Here is the call graph for this function:



10.11.3.56 fdJzdx()

```
void fdJzdx (
            std::vector< realtype > * dJzdx,
            const int nroots,
            realtype t,
            const ExpData * edata,
            const ReturnData * rdata )
```

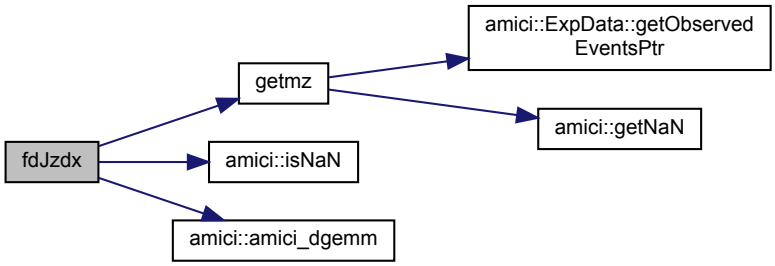
Sensitivity of event-resolved measurement negative log-likelihood Jz w.r.t. state variables

Parameters

dJzdx	pointer to vector with values of state derivative of Jz
nroots	event index
t	current timepoint
edata	pointer to experimental data instance
rdata	pointer to return data instance

Definition at line 200 of file model.cpp.

Here is the call graph for this function:



10.11.3.57 initialize()

```
void initialize (
            AmiVector * x,
            AmiVector * dx )
```

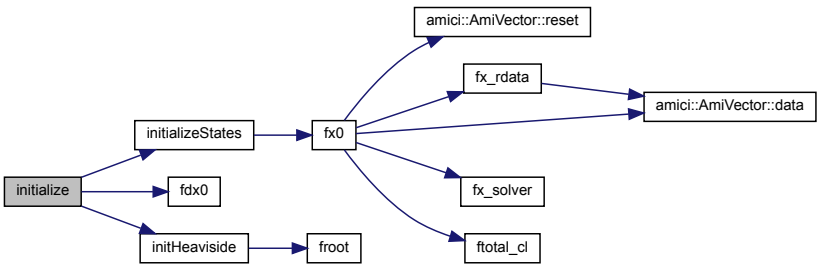
initialization of model properties

Parameters

x	pointer to state variables
dx	pointer to time derivative of states (DAE only)

Definition at line 223 of file model.cpp.

Here is the call graph for this function:



10.11.3.58 initializeStates()

```
void initializeStates (
            AmiVector * x )
```

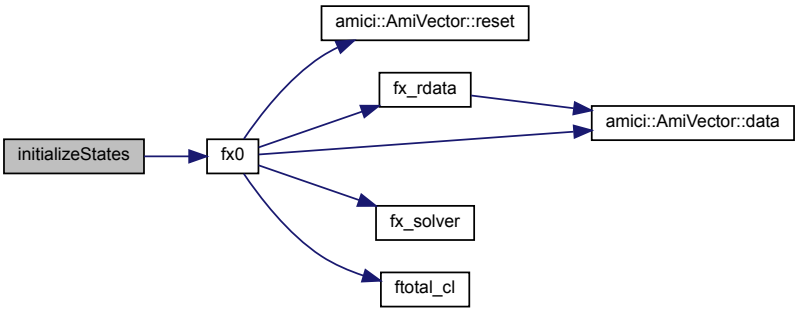
initialization of initial states

Parameters

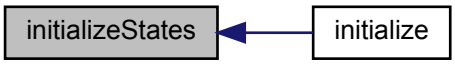
x	pointer to state variables

Definition at line 234 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.59 initHeaviside()

```
void initHeaviside (
            AmiVector * x,
            AmiVector * dx )
```

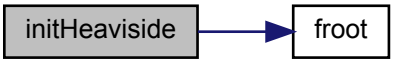
initHeaviside initialises the heaviside variables h at the intial time t0 heaviside variables activate/deactivate on event occurences

Parameters

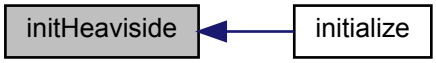
x	pointer to state variables
dx	pointer to time derivative of states (DAE only)

Definition at line 245 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.60 nplist()

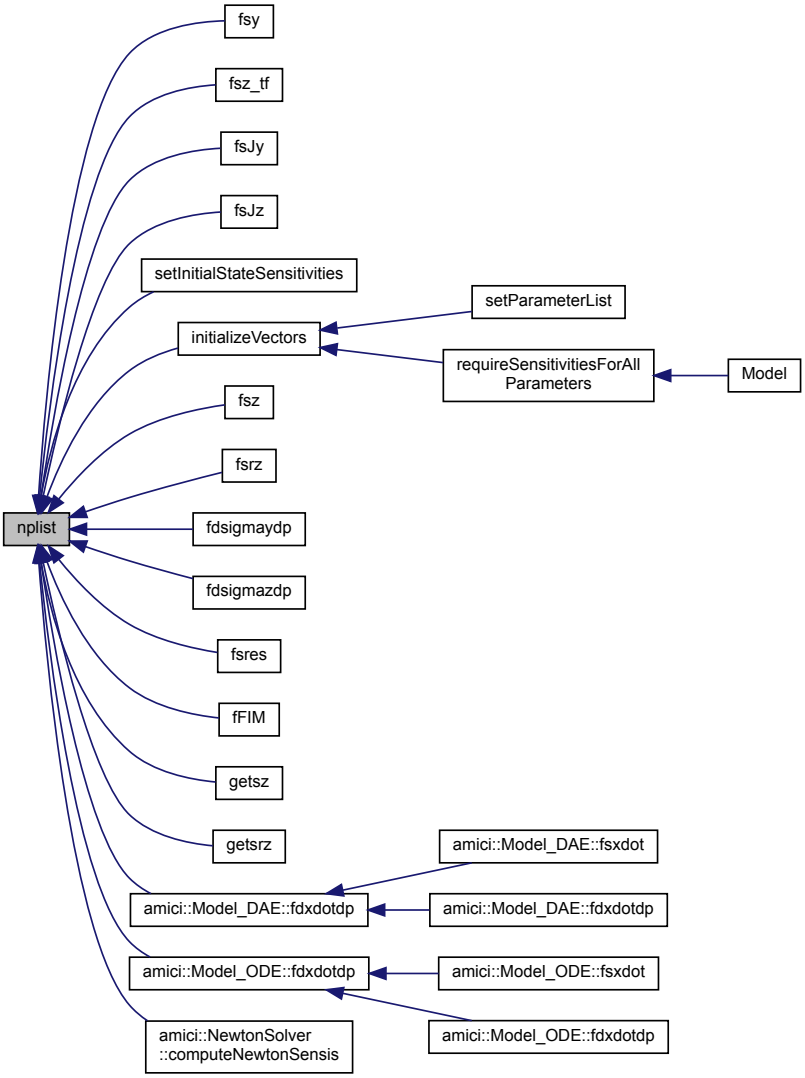
```
int nplist ( ) const
```

Returns

length of sensitivity index vector

Definition at line 262 of file model.cpp.

Here is the caller graph for this function:



10.11.3.61 np()

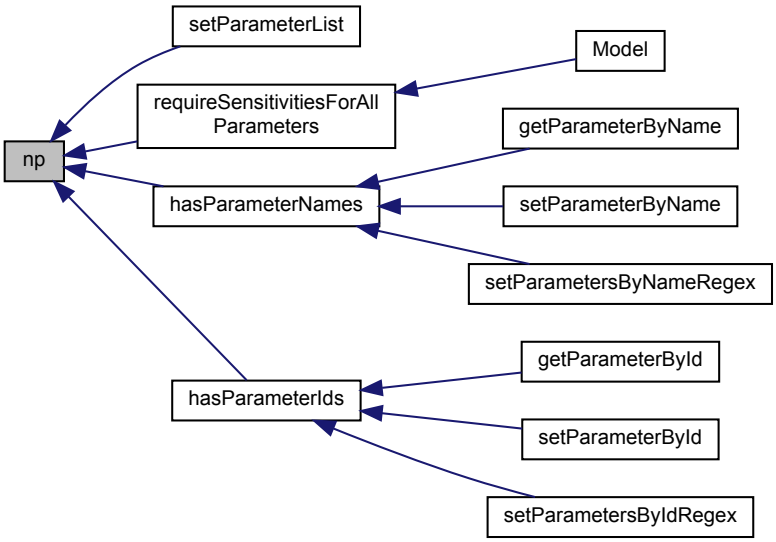
```
int np ( ) const
```

Returns

length of parameter vector

Definition at line 266 of file model.cpp.

Here is the caller graph for this function:



10.11.3.62 nk()

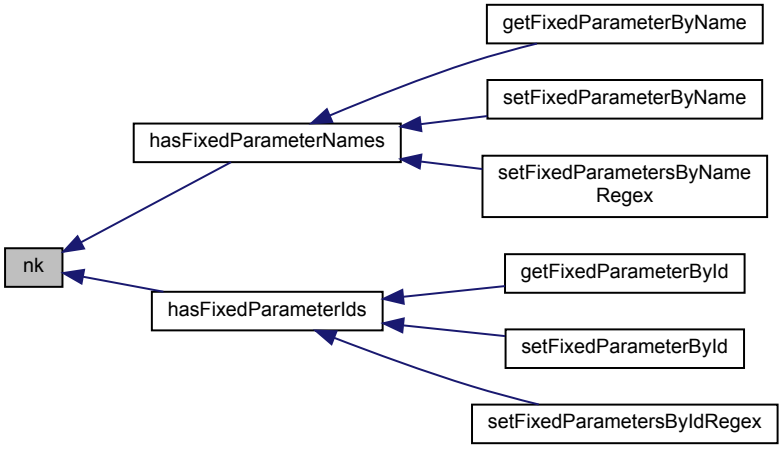
```
int nk ( ) const
```

Returns

length of constant vector

Definition at line 270 of file model.cpp.

Here is the caller graph for this function:



10.11.3.63 ncl()

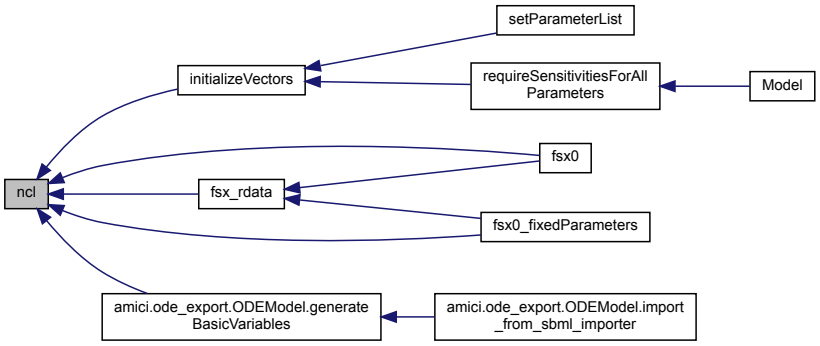
```
int ncl ( ) const
```

Returns

difference between nx_rdata and nx_solver

Definition at line 592 of file model.h.

Here is the caller graph for this function:



10.11.3.64 k()

```
const double * k ( ) const
```

Returns

pointer to constants array

Definition at line 274 of file model.cpp.

Here is the caller graph for this function:

10.11.3.65 nMaxEvent()

```
int nMaxEvent ( ) const
```

Returns

maximum number of events that may occur for each type

Definition at line 278 of file model.cpp.

10.11.3.66 setNMaxEvent()

```
void setNMaxEvent (
            int nmaxevent )
```

Parameters

nmaxevent	maximum number of events that may occur for each type

Definition at line 282 of file model.cpp.

10.11.3.67 nt()

```
int nt ( ) const
```

Returns

number of timepoints

Definition at line 286 of file model.cpp.

10.11.3.68 getParameterScale()

```
const std::vector< ParameterScaling > & getParameterScale ( ) const
```

Returns

vector of parameter scale

Definition at line 290 of file model.cpp.

10.11.3.69 setParameterScale() [1/2]

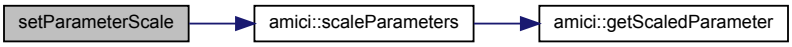
```
void setParameterScale (
            ParameterScaling pscale )
```

Parameters

pscale	scalar parameter scale for all parameters

Definition at line 294 of file model.cpp.

Here is the call graph for this function:



10.11.3.70 setParameterScale() [2/2]

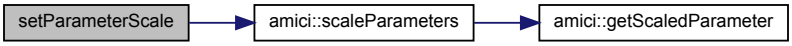
```
void setParameterScale (
            const std::vector< ParameterScaling > & pscale )
```

Parameters

pscale	vector of parameter scales

Definition at line 299 of file model.cpp.

Here is the call graph for this function:



10.11.3.71 getParameters()

```
std::vector< realtype > const & getParameters ( ) const
```

Returns

The user-set parameters (see also getUnscaledParameters)

Definition at line 306 of file model.cpp.

10.11.3.72 setParameters()

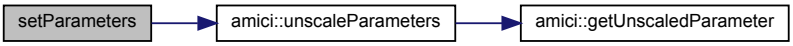
```
void setParameters (
            std::vector< realtype > const & p )
```

Parameters

p	vector of parameters

Definition at line 393 of file model.cpp.

Here is the call graph for this function:



10.11.3.73 getUnscaledParameters()

```
const std::vector< realtype > & getUnscaledParameters ( ) const
```

Returns

unscaled parameters

Definition at line 455 of file model.cpp.

10.11.3.74 getFixedParameters()

```
const std::vector< realtype > & getFixedParameters ( ) const
```

Returns

vector of fixed parameters

Definition at line 459 of file model.cpp.

10.11.3.75 setFixedParameters()

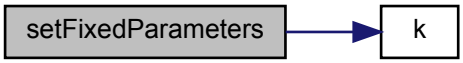
```
void setFixedParameters (
            std::vector< realtype > const & k )
```

Parameters

k	vector of fixed parameters

Definition at line 485 of file model.cpp.

Here is the call graph for this function:



10.11.3.76 getFixedParameterById()

```
realtype getFixedParameterById (
            std::string const & par_id ) const
```

Parameters

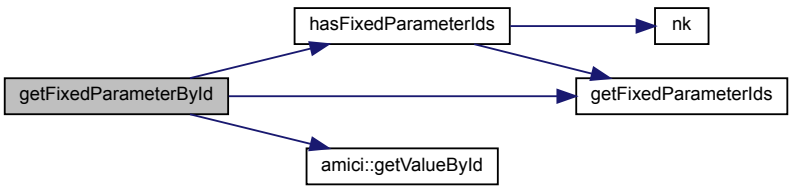
par_id	parameter id

Returns

parameter value

Definition at line 463 of file model.cpp.

Here is the call graph for this function:



10.11.3.77 getFixedParameterByName()

```
realtype getFixedParameterByName (
            std::string const & par_name ) const
```

Parameters

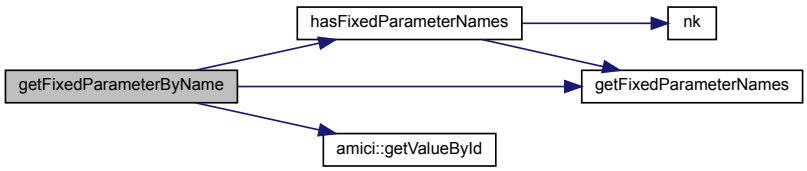
par_name	parameter name

Returns

parameter value

Definition at line 474 of file model.cpp.

Here is the call graph for this function:



10.11.3.78 setFixedParameterById()

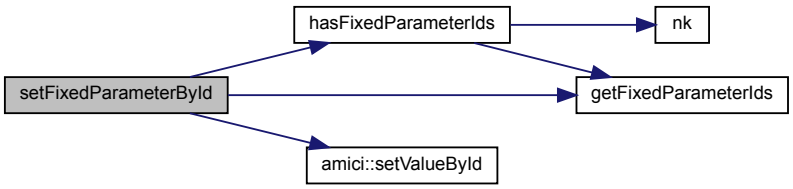
```
void setFixedParameterById (
            std::string const & par_id,
            realtype value )
```

Parameters

par↩ _id	fixed parameter id
value	fixed parameter value

Definition at line 491 of file model.cpp.

Here is the call graph for this function:



10.11.3.79 setFixedParametersByIdRegex()

```
int setFixedParametersByIdRegex (
            std::string const & par_id_regex,
            realtype value )
```

Parameters

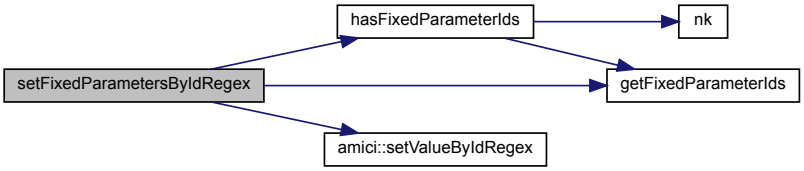
par_id_regex	fixed parameter name regex
value	fixed parameter value

Returns

number of fixed parameter ids that matched the regex

Definition at line 503 of file model.cpp.

Here is the call graph for this function:



10.11.3.80 setFixedParameterByName()

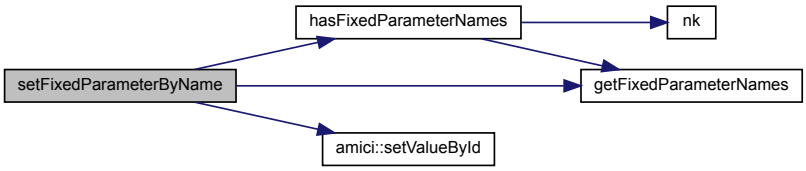
```
void setFixedParameterByName (
            std::string const & par_name,
            realtype value )
```

Parameters

par_name	fixed parameter id
value	fixed parameter value

Definition at line 515 of file model.cpp.

Here is the call graph for this function:



10.11.3.81 setFixedParametersByNameRegex()

```
int setFixedParametersByNameRegex (
            std::string const & par_name_regex,
            realtype value )
```

Parameters

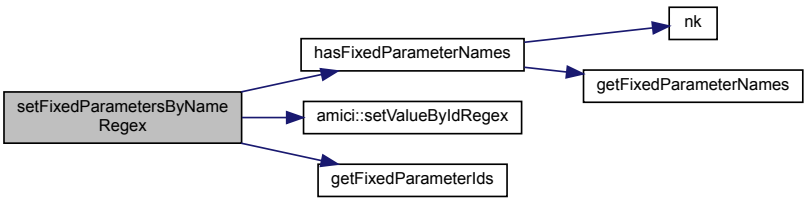
par_name_regex	fixed parameter name regex
value	fixed parameter value

Returns

number of fixed parameter names that matched the regex

Definition at line 527 of file model.cpp.

Here is the call graph for this function:



10.11.3.82 getTimepoints()

```
std::vector< realtype > const & getTimepoints ( ) const
```

Returns

timepoint vector

Definition at line 539 of file model.cpp.

10.11.3.83 setTimepoints()

```
void setTimepoints (
            std::vector< realtype > const & ts )
```

Parameters

ts	timepoint vector

Definition at line 543 of file model.cpp.

10.11.3.84 getStateIsNonNegative()

```
std::vector< bool > const & getStateIsNonNegative ( ) const
```

Returns

vector of flags

Definition at line 549 of file model.cpp.

10.11.3.85 setStateIsNonNegative()

```
void setStateIsNonNegative (
            std::vector< bool > const & stateIsNonNegative )
```

Parameters

stateIsNonNegative	vector of flags

Definition at line 553 of file model.cpp.

10.11.3.86 t()

```
double t (
            int idx ) const
```

Parameters

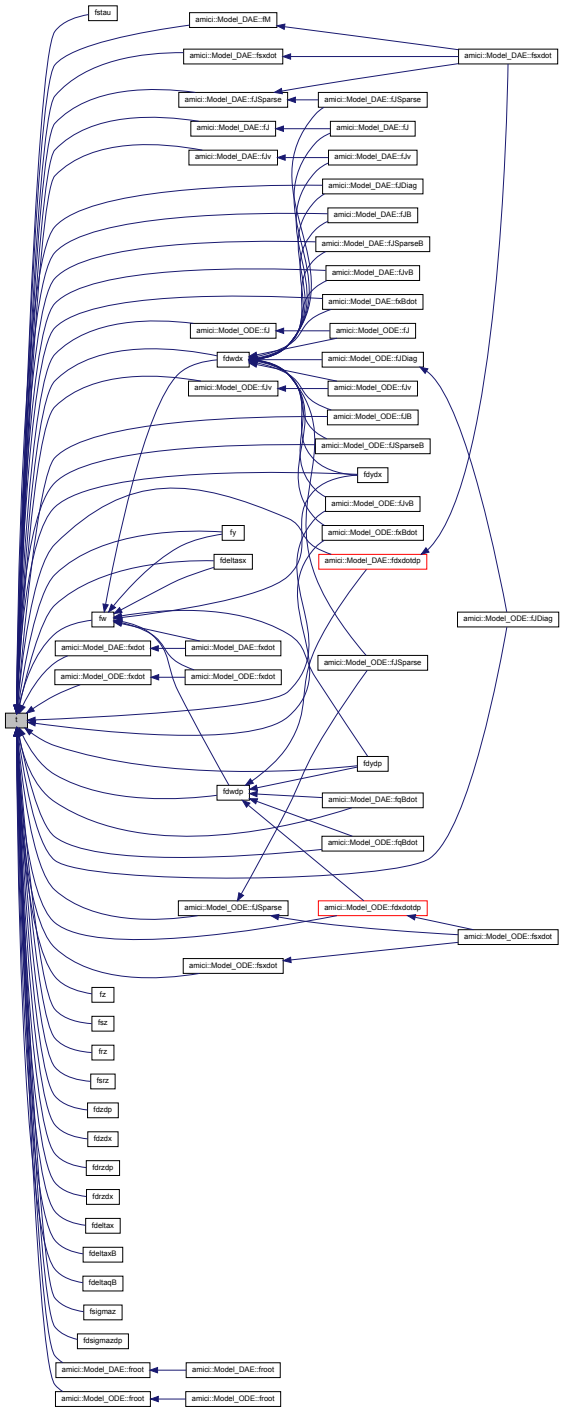
idx	timepoint index

Returns

timepoint

Definition at line 568 of file model.cpp.

Here is the caller graph for this function:



10.11.3.87 getParameterList()

```
const std::vector< int > & getParameterList ( ) const
```

Returns

list of parameter indices

Definition at line 572 of file model.cpp.

10.11.3.88 setParameterList()

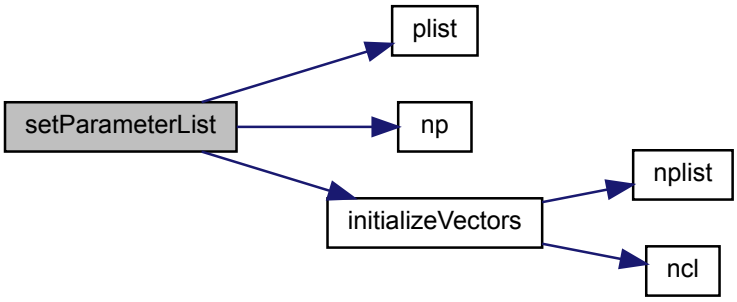
```
void setParameterList (
            std::vector< int > const & plist )
```

Parameters

plist	list of parameter indices

Definition at line 576 of file model.cpp.

Here is the call graph for this function:



10.11.3.89 getInitialStates()

```
std::vector< realtype > const & getInitialStates ( ) const
```

Returns

initial state vector

Definition at line 585 of file model.cpp.

10.11.3.90 setInitialStates()

```
void setInitialStates (
            std::vector< realtype > const & x0 )
```

Parameters

x0	initial state vector

Definition at line 589 of file model.cpp.

10.11.3.91 getInitialStateSensitivities()

```
const std::vector< realtype > & getInitialStateSensitivities ( ) const
```

Returns

vector of initial state sensitivities

Definition at line 601 of file model.cpp.

10.11.3.92 setInitialStateSensitivities()

```
void setInitialStateSensitivities (
            std::vector< realtype > const & sx0 )
```

Parameters

sx0	vector of initial state sensitivities

Definition at line 605 of file model.cpp.

Here is the call graph for this function:

10.11.3.93 t0()

```
double t0 ( ) const
```

Returns

simulation start time

Definition at line 617 of file model.cpp.

Here is the caller graph for this function:

10.11.3.94 setT0()

```
void setT0 (
            double t0 )
```

Parameters

t0	simulation start time

Definition at line 621 of file model.cpp.

Here is the call graph for this function:

10.11.3.95 plist()

```
int plist (
            int pos ) const
```

Parameters

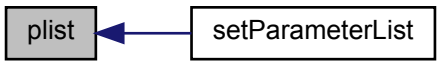
pos	index

Returns

entry

Definition at line 625 of file model.cpp.

Here is the caller graph for this function:



10.11.3.96 fw() [1/2]

```
void fw (
            const realtype t,
            const realtype * x )
```

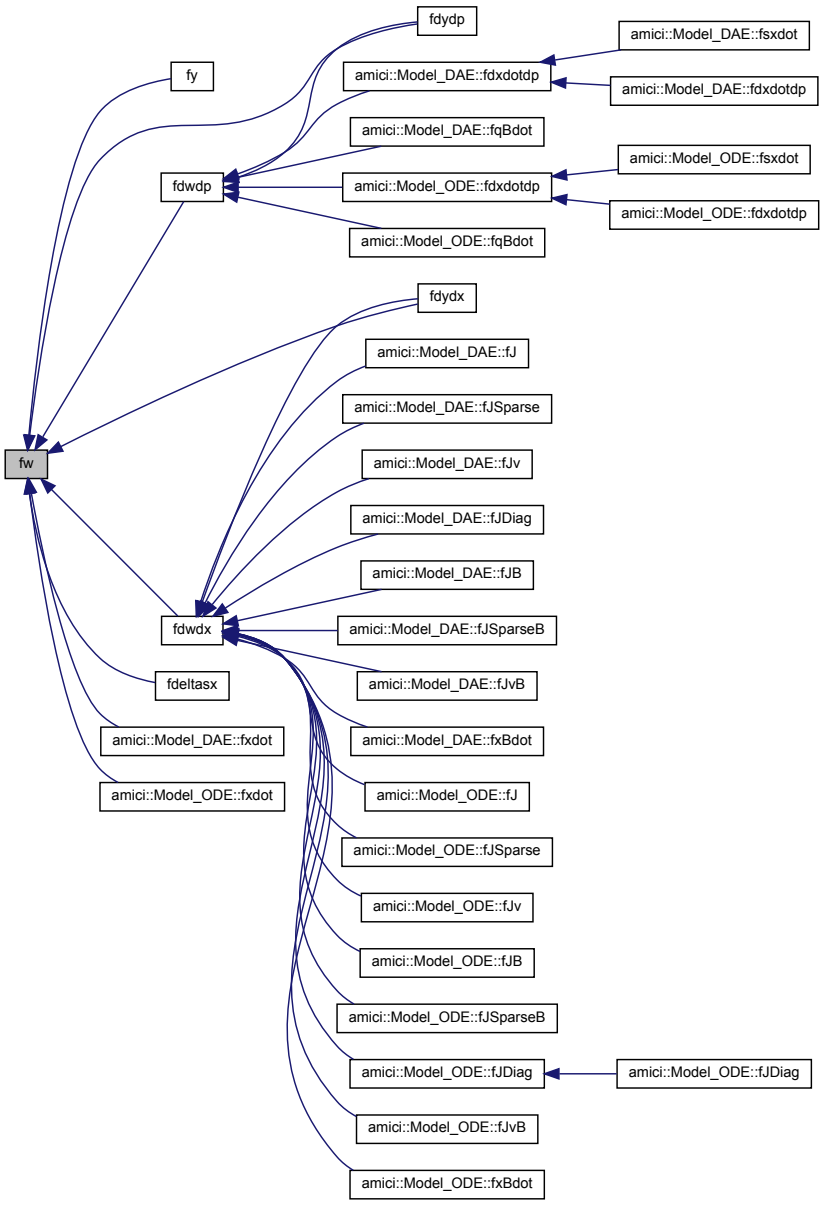
Parameters

t	timepoint
x	array with the states

Definition at line 1205 of file model.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



10.11.3.97 fdwdp() [1/2]

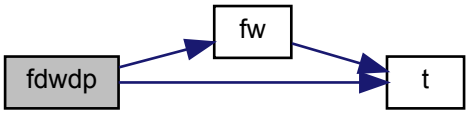
```
void fdwdp (
            const realtype t,
            const realtype * x )
```

Parameters

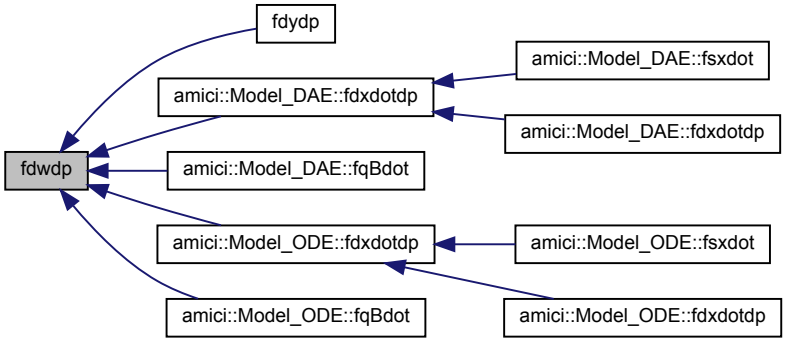
t	timepoint
x	array with the states

Definition at line 1210 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.98 fdwdx() [1/2]

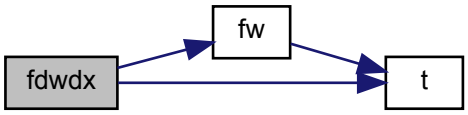
```
void fdwdx (
            const realtype t,
            const realtype * x )
```

Parameters

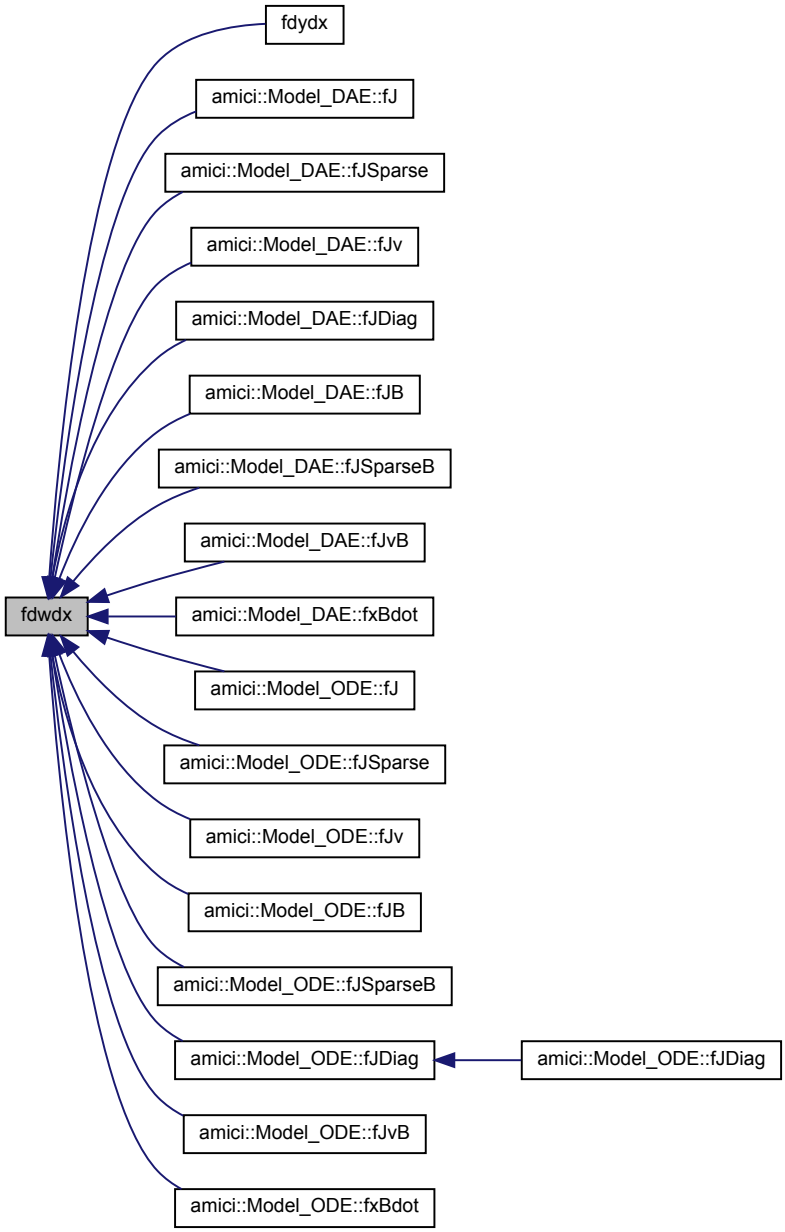
t	timepoint
x	array with the states

Definition at line 1216 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.99 fres()

```
void fres (
            const int it,
            ReturnData * rdata,
            const ExpData * edata )
```

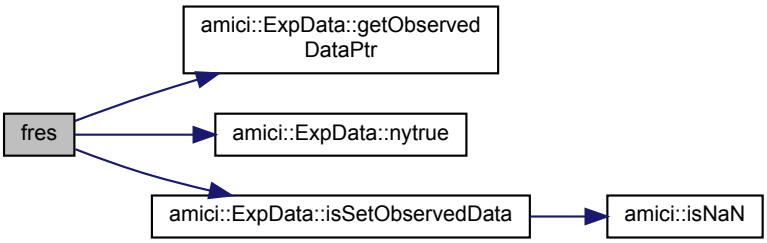
residual function

Parameters

it	time index
rdata	ReturnData instance to which result will be written
edata	ExpData instance containing observable data

Definition at line 1222 of file model.cpp.

Here is the call graph for this function:



10.11.3.100 fchi2()

```
void fchi2 (
            const int it,
            ReturnData * rdata )
```

chi-squared function

Parameters

it	time index
rdata	ReturnData instance to which result will be written

Definition at line 1237 of file model.cpp.

10.11.3.101 fsres()

```
void fsres (
            const int it,
            ReturnData * rdata,
            const ExpData * edata )
```

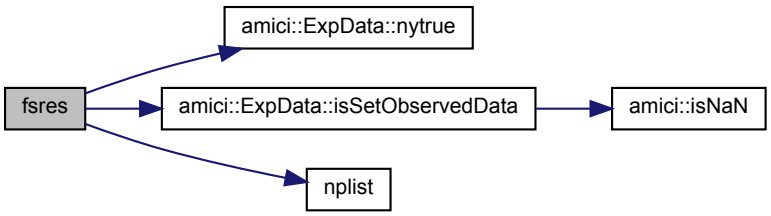
residual sensitivity function

Parameters

it	time index
rdata	ReturnData instance to which result will be written
edata	ExpData instance containing observable data

Definition at line 1247 of file model.cpp.

Here is the call graph for this function:



10.11.3.102 fFIM()

```
void fFIM (
            const int it,
            ReturnData * rdata )
```

fisher information matrix function

Parameters

it	time index
rdata	ReturnData instance to which result will be written

Definition at line 1263 of file model.cpp.

Here is the call graph for this function:

10.11.3.103 updateHeaviside()

```
void updateHeaviside (
            const std::vector< int > & rootsfound )
```

updateHeaviside updates the heaviside variables h on event occurences

Parameters

rootsfound	provides the direction of the zero-crossing, so adding it will give the right update to the heaviside variables (zero if no root was found)

Definition at line 1279 of file model.cpp.

10.11.3.104 updateHeavisideB()

```
void updateHeavisideB (
            const int * rootsfound )
```

updateHeavisideB updates the heaviside variables h on event occurences in the backward problem

Parameters

rootsfound	provides the direction of the zero-crossing, so adding it will give the right update to the heaviside variables (zero if no root was found)

Definition at line 1285 of file model.cpp.

10.11.3.105 gett()

```
realtype gett (
            const int it,
            const ReturnData * rdata ) const
```

get current timepoint from index

Parameters

it	timepoint index
rdata	pointer to return data instance

Returns

current timepoint

Definition at line 1304 of file model.cpp.

10.11.3.106 checkFinite()

```
int checkFinite (
            const int N,
            const realtype * array,
            const char * fun ) const
```

Parameters

N	number of datapoints in array
array	arrays of values
fun	name of the fucntion that generated the values

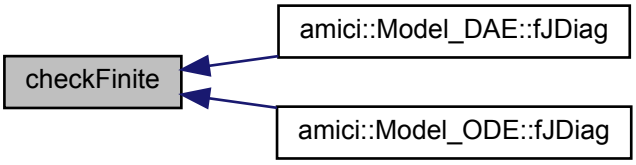
Returns

AMICI_RECOVERABLE_ERROR if a NaN/Inf value was found, AMICI_SUCCESS otherwise

Definition at line 1332 of file model.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



10.11.3.107 hasParameterNames()

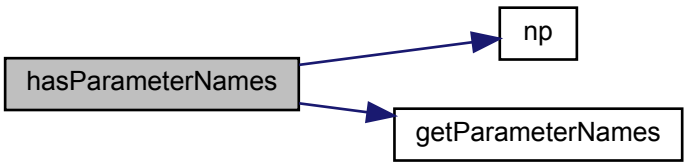
```
virtual bool hasParameterNames ( ) const  [virtual]
```

Returns

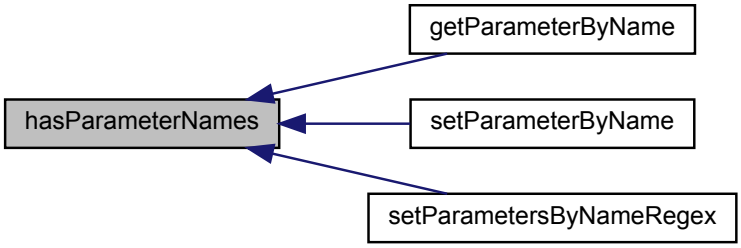
boolean indicating whether parameter names were set

Definition at line 911 of file model.h.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.108 getParameterNames()

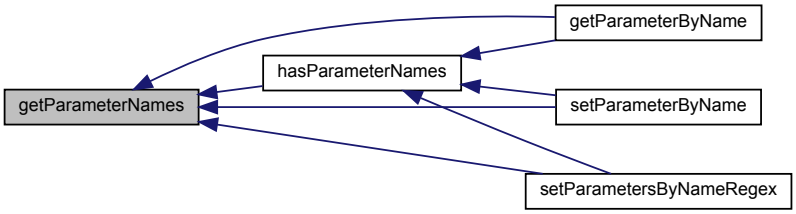
```
virtual std::vector<std::string> getParameterNames ( ) const  [virtual]
```

Returns

the names

Definition at line 917 of file model.h.

Here is the caller graph for this function:



10.11.3.109 hasStateNames()

```
virtual bool hasStateNames ( ) const  [virtual]
```

Returns

boolean indicating whether state names were set

Definition at line 923 of file model.h.

Here is the call graph for this function:

10.11.3.110 getStateNames()

```
virtual std::vector<std::string> getStateNames ( ) const  [virtual]
```

Returns

the names

Definition at line 929 of file model.h.

Here is the caller graph for this function:

10.11.3.111 hasFixedParameterNames()

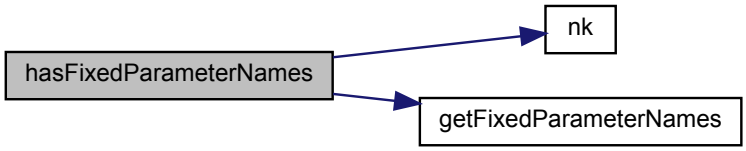
```
virtual bool hasFixedParameterNames ( ) const  [virtual]
```

Returns

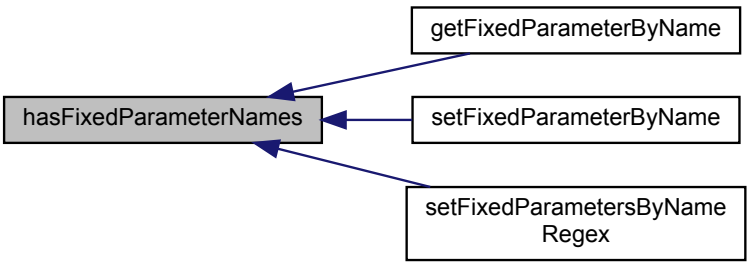
boolean indicating whether fixed parameter names were set

Definition at line 935 of file model.h.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.112 getFixedParameterNames()

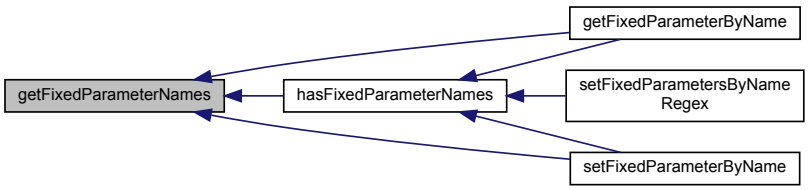
```
virtual std::vector<std::string> getFixedParameterNames ( ) const  [virtual]
```

Returns

the names

Definition at line 941 of file model.h.

Here is the caller graph for this function:



10.11.3.113 hasObservableNames()

```
virtual bool hasObservableNames ( ) const  [virtual]
```

Returns

boolean indicating whether observabke names were set

Definition at line 947 of file model.h.

Here is the call graph for this function:

10.11.3.114 getObservableNames()

```
virtual std::vector<std::string> getObservableNames ( ) const  [virtual]
```

Returns

the names

Definition at line 953 of file model.h.

Here is the caller graph for this function:

10.11.3.115 hasParameterIds()

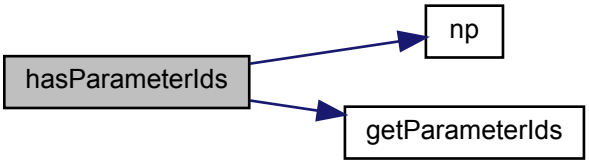
```
virtual bool hasParameterIds ( ) const  [virtual]
```

Returns

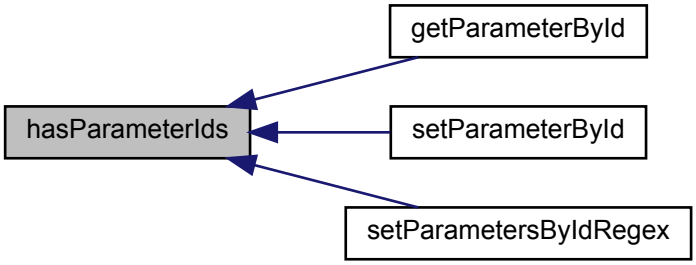
boolean indicating whether parameter ids were set

Definition at line 959 of file model.h.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.116 getParameterIds()

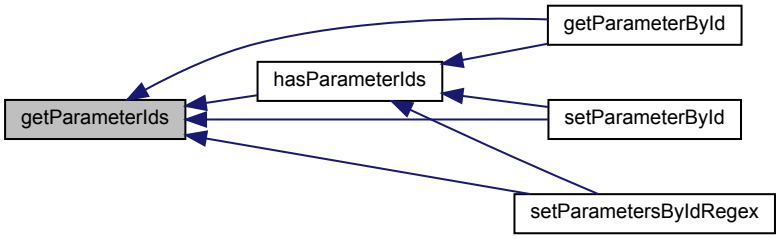
```
virtual std::vector<std::string> getParameterIds ( ) const  [virtual]
```

Returns

the ids

Definition at line 965 of file model.h.

Here is the caller graph for this function:



10.11.3.117 getParameterById()

```
realtype getParameterById (
            std::string const & par_id ) const
```

Parameters

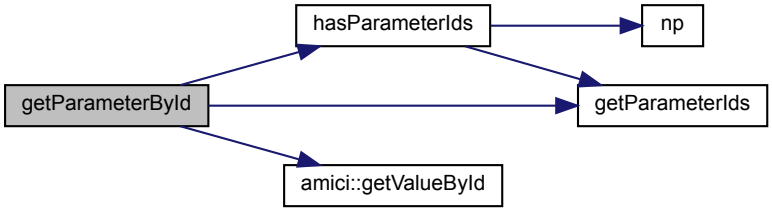
par↩ _id	parameter id

Returns

parameter value

Definition at line 377 of file model.cpp.

Here is the call graph for this function:



10.11.3.118 getParameterByName()

```
realtype getParameterByName (
            std::string const & par_name ) const
```

Parameters

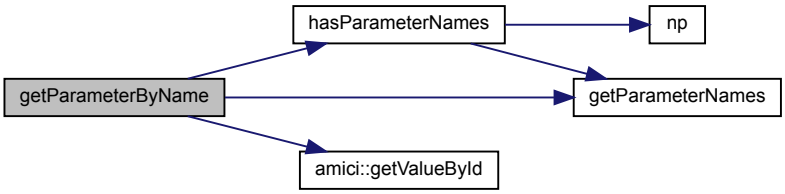
par_name	parameter name

Returns

parameter value

Definition at line 383 of file model.cpp.

Here is the call graph for this function:



10.11.3.119 setParameterById()

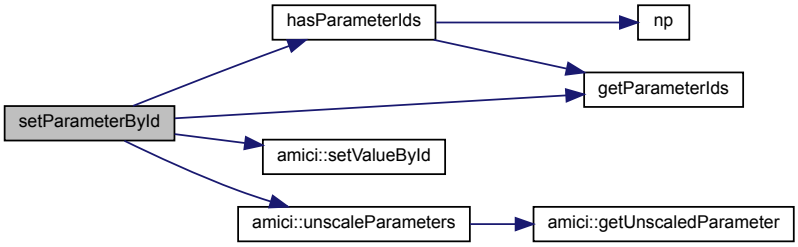
```
void setParameterById (
            std::string const & par_id,
            realtype value )
```

Parameters

par_id	parameter id
value	parameter value

Definition at line 401 of file model.cpp.

Here is the call graph for this function:



10.11.3.120 setParametersByIdRegex()

```
int setParametersByIdRegex (
            std::string const & par_id_regex,
            realtype value )
```

Parameters

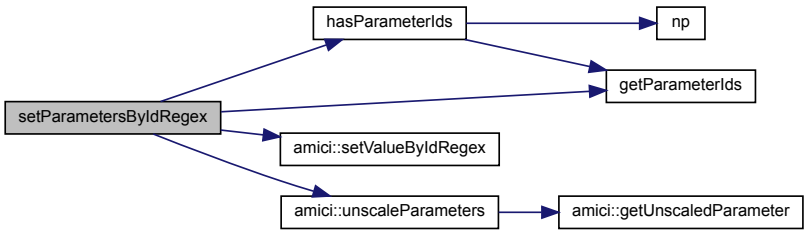
par_id_regex	parameter id regex
value	parameter value

Returns

number of parameter ids that matched the regex

Definition at line 414 of file model.cpp.

Here is the call graph for this function:



10.11.3.121 setParameterByName()

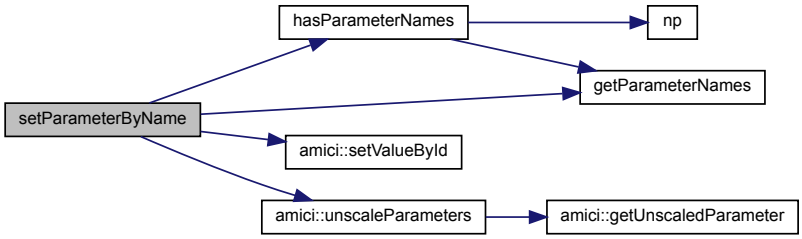
```
void setParameterByName (
            std::string const & par_name,
            realtype value )
```

Parameters

par_name	parameter name
value	parameter value

Definition at line 427 of file model.cpp.

Here is the call graph for this function:



10.11.3.122 setParametersByNameRegex()

```
int setParametersByNameRegex (
            std::string const & par_name_regex,
            realtype value )
```

Parameters

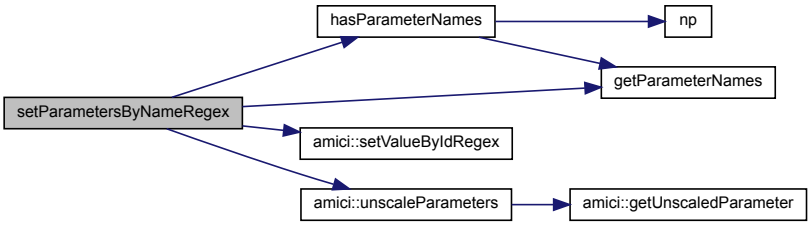
par_name_regex	parameter name regex
value	parameter value

Returns

number of fixed parameter names that matched the regex

Definition at line 440 of file model.cpp.

Here is the call graph for this function:



10.11.3.123 hasStateIds()

```
virtual bool hasStateIds ( ) const  [virtual]
```

Returns

Definition at line 1017 of file model.h.

Here is the call graph for this function:

10.11.3.124 getStateIds()

```
virtual std::vector<std::string> getStateIds ( ) const  [virtual]
```

Returns

the ids

Definition at line 1023 of file model.h.

Here is the caller graph for this function:

10.11.3.125 hasFixedParameterIds()

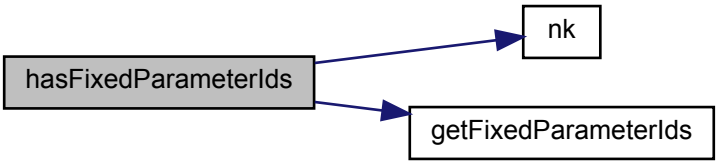
```
virtual bool hasFixedParameterIds ( ) const  [virtual]
```

Returns

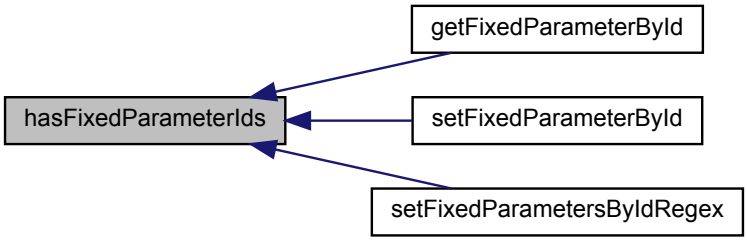
boolean indicating whether fixed parameter ids were set

Definition at line 1031 of file model.h.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.126 getFixedParameterIds()

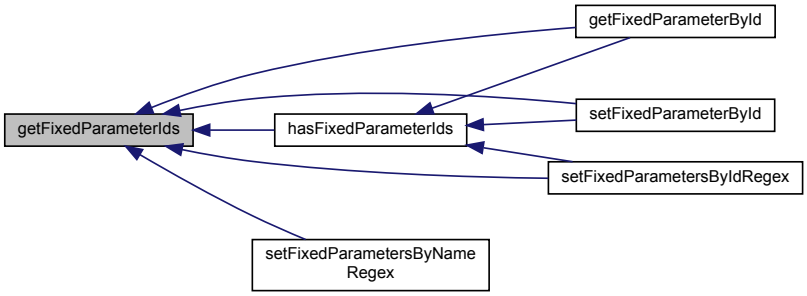
```
virtual std::vector<std::string> getFixedParameterIds ( ) const  [virtual]
```

Returns

the ids

Definition at line 1037 of file model.h.

Here is the caller graph for this function:



10.11.3.127 hasObservableIds()

```
virtual bool hasObservableIds ( ) const  [virtual]
```

Returns

boolean indicating whether observale ids were set

Definition at line 1045 of file model.h.

Here is the call graph for this function:

10.11.3.128 getObservableIds()

```
virtual std::vector<std::string> getObservableIds ( ) const  [virtual]
```

Returns

the ids

Definition at line 1051 of file model.h.

Here is the caller graph for this function:

10.11.3.129 setSteadyStateSensitivityMode()

```
void setSteadyStateSensitivityMode (
            const SteadyStateSensitivityMode mode )
```

Parameters

mode	steadyStateSensitivityMode

Definition at line 1059 of file model.h.

10.11.3.130 getSteadyStateSensitivityMode()

```
SteadyStateSensitivityMode getSteadyStateSensitivityMode ( ) const
```

Returns

flag value

Definition at line 1067 of file model.h.

10.11.3.131 setReinitializeFixedParameterInitialStates()

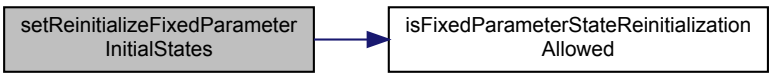
```
void setReinitializeFixedParameterInitialStates (
            bool flag )
```

Parameters

flag	true/false

Definition at line 1076 of file model.h.

Here is the call graph for this function:



10.11.3.132 getReinitializeFixedParameterInitialStates()

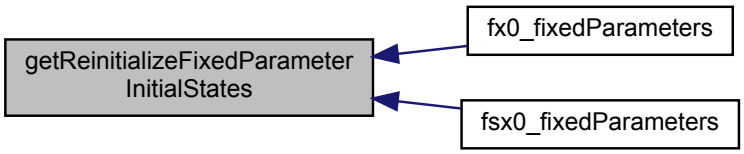
```
bool getReinitializeFixedParameterInitialStates ( ) const
```

Returns

flag true/false

Definition at line 1090 of file model.h.

Here is the caller graph for this function:



10.11.3.133 fx_rdata() [2/2]

```
virtual void fx_rdata (
            realtype * x_rdata,
            const realtype * x_solver,
            const realtype * tcl )  [protected], [virtual]
```

model specific implementation of fx_rdata

Parameters

x_rdata	state variables with conservation laws expanded
x_solver	state variables with conservation laws applied
tcl	total abundances for conservation laws

Definition at line 1172 of file model.h.

10.11.3.134 fsx_rdata() [2/2]

```
virtual void fsx_rdata (
            realtype * sx_rdata,
            const realtype * sx_solver,
            const realtype * stcl,
            const int ip )  [protected], [virtual]
```

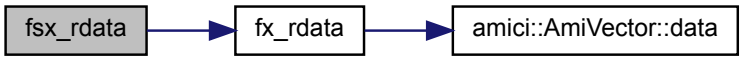
model specific implementation of fsx_solver

Parameters

sx_rdata	state sensitivity variables with conservation laws expanded
sx_solver	state sensitivity variables with conservation laws applied
stcl	sensitivities of total abundances for conservation laws
ip	sensitivity index

Definition at line 1189 of file model.h.

Here is the call graph for this function:



10.11.3.135 fx_solver()

```
virtual void fx_solver (
            realtype * x_solver,
            const realtype * x_rdata )  [protected], [virtual]
```

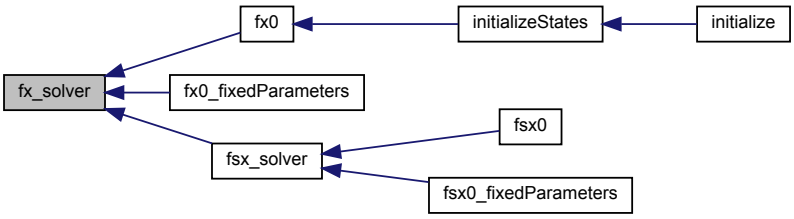
model specific implementation of fx_solver

Parameters

x_solver	state variables with conservation laws applied
x_rdata	state variables with conservation laws expanded

Definition at line 1198 of file model.h.

Here is the caller graph for this function:



10.11.3.136 fsx_solver()

```
virtual void fsx_solver (
            realtype * sx_solver,
            const realtype * sx_rdata )  [protected], [virtual]
```

model specific implementation of fsx_solver

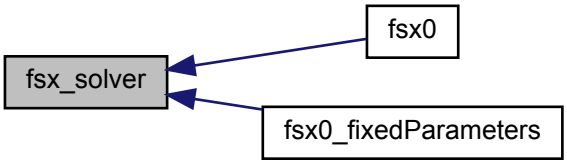
Parameters

sx_rdata	state sensitivity variables with conservation laws expanded
sx_solver	state sensitivity variables with conservation laws applied

Definition at line 1211 of file model.h.

Here is the call graph for this function:

Here is the caller graph for this function:



10.11.3.137 ftotal_cl()

```
virtual void ftotal_cl (
            realtype * total_cl,
            const realtype * x_rdata )  [protected], [virtual]
```

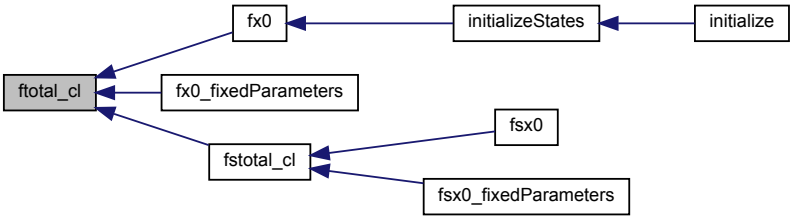
model specific implementation of ftotal_cl

Parameters

total_cl	total abundances of conservation laws
x_rdata	state variables with conservation laws expanded

Definition at line 1222 of file model.h.

Here is the caller graph for this function:



10.11.3.138 fstotal_cl()

```
virtual void fstotal_cl (
            realtype * stotal_cl,
            const realtype * sx_rdata,
            const int ip )  [protected], [virtual]
```

model specific implementation of fstotal_cl

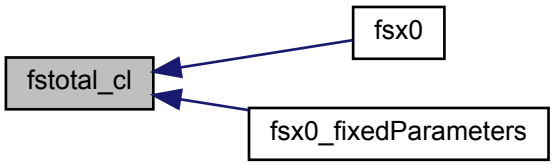
Parameters

stotal↩ _cl	sensitivites for the total abundances of conservation laws
sx_rdata	state sensitivity variables with conservation laws expanded
ip	sensitivity index

Definition at line 1236 of file model.h.

Here is the call graph for this function:

Here is the caller graph for this function:



10.11.3.139 fx0() [2/2]

```
virtual void fx0 (
            realtype * x0,
            const realtype t,
            const realtype * p,
            const realtype * k )  [protected], [virtual]
```

model specific implementation of fx0

Parameters

x0	initial state
t	initial time
p	parameter vector
k	constant vector

Definition at line 1250 of file model.h.

10.11.3.140 fx0_fixedParameters() [2/2]

```
virtual void fx0_fixedParameters (
            realtype * x0,
            const realtype t,
            const realtype * p,
            const realtype * k )  [protected], [virtual]
```

model specific implementation of fx0_fixedParameters

Parameters

x0	initial state
t	initial time
p	parameter vector
k	constant vector

Definition at line 1260 of file model.h.

10.11.3.141 fsx0_fixedParameters() [2/2]

```
virtual void fsx0_fixedParameters (
            realtype * sx0,
            const realtype t,
            const realtype * x0,
            const realtype * p,
            const realtype * k,
            const int ip )  [protected], [virtual]
```

model specific implementation of fsx0_fixedParameters

Parameters

sx0	initial state sensitivities
t	initial time
x0	initial state
p	parameter vector
k	constant vector
ip	sensitivity index

Definition at line 1271 of file model.h.

10.11.3.142 fsx0() [2/2]

```
virtual void fsx0 (
            realtype * sx0,
            const realtype t,
            const realtype * x0,
            const realtype * p,
            const realtype * k,
            const int ip )  [protected], [virtual]
```

model specific implementation of fsx0

Parameters

sx0	initial state sensitivities
t	initial time
x0	initial state
p	parameter vector
k	constant vector
ip	sensitivity index

Definition at line 1282 of file model.h.

10.11.3.143 fstau() [2/2]

```
virtual void fstau (
            realtype * stau,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * sx,
            const int ip,
            const int ie )  [protected], [virtual]
```

model specific implementation of fstau

Parameters

stau	total derivative of event timepoint
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
sx	current state sensitivity
ip	sensitivity index
ie	event index

Definition at line 1297 of file model.h.

10.11.3.144 fy() [2/2]

```
virtual void fy (
            realtype * y,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * w )  [protected], [virtual]
```

model specific implementation of fy

Parameters

y	model output at current timepoint
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
w	repeating elements vector

Definition at line 1310 of file model.h.

10.11.3.145 fdydp() [2/2]

```
virtual void fdydp (
            realtype * dydp,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ip,
            const realtype * w,
            const realtype * dwdp )  [protected], [virtual]
```

model specific implementation of fdydp

Parameters

dydp	partial derivative of observables y w.r.t. model parameters p
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
ip	parameter index w.r.t. which the derivative is requested
w	repeating elements vector
dwdp	Recurring terms in xdot, parameter derivative

Definition at line 1325 of file model.h.

10.11.3.146 fdydx() [2/2]

```
virtual void fdydx (
            realtype * dydx,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation of fdydx

Parameters

dydx	partial derivative of observables y w.r.t. model states x
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
w	repeating elements vector
dwdx	Recurring terms in xdot, state derivative

Definition at line 1339 of file model.h.

10.11.3.147 fz() [2/2]

```
virtual void fz (
            realtype * z,
            const int ie,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h )  [protected], [virtual]
```

model specific implementation of fz

Parameters

z	value of event output
ie	event index
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector

Definition at line 1352 of file model.h.

10.11.3.148 fsz() [2/2]

```
virtual void fsz (
            realtype * sz,
            const int ie,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * sx,
            const int ip )  [protected], [virtual]
```

model specific implementation of fsz

Parameters

sz	Sensitivity of rz, total derivative
ie	event index
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
sx	current state sensitivity
ip	sensitivity index

Definition at line 1367 of file model.h.

10.11.3.149 frz() [2/2]

```
virtual void frz (
            realtype * rz,
            const int ie,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h )  [protected], [virtual]
```

model specific implementation of frz

Parameters

rz	value of root function at current timepoint (non-output events not included)
ie	event index
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector

Definition at line 1380 of file model.h.

10.11.3.150 fsrz() [2/2]

```
virtual void fsrz (
            realtype * srz,
            const int ie,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * sx,
            const int ip )  [protected], [virtual]
```

model specific implementation of fsrz

Parameters

srz	Sensitivity of rz, total derivative
ie	event index
t	current time
x	current state
p	parameter vector
k	constant vector
sx	current state sensitivity
h	heavyside vector
ip	sensitivity index

Definition at line 1395 of file model.h.

10.11.3.151 fdzdp() [2/2]

```
virtual void fdzdp (
            realtype * dzdp,
            const int ie,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ip )  [protected], [virtual]
```

model specific implementation of fdzdp

Parameters

dzdp	partial derivative of event-resolved output z w.r.t. model parameters p
ie	event index
t	current time

Parameters

x	current state
p	parameter vector
k	constant vector
h	heavyside vector
ip	parameter index w.r.t. which the derivative is requested

Definition at line 1409 of file model.h.

10.11.3.152 fdzdx() [2/2]

```
virtual void fdzdx (
            realtype * dzdx,
            const int ie,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h )  [protected], [virtual]
```

model specific implementation of fdzdx

Parameters

dzdx	partial derivative of event-resolved output z w.r.t. model states x
ie	event index
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector

Definition at line 1422 of file model.h.

10.11.3.153 fdrzdp() [2/2]

```
virtual void fdrzdp (
            realtype * drzdp,
            const int ie,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ip )  [protected], [virtual]
```

model specific implementation of fdrzdp

Parameters

drzdp	partial derivative of root output rz w.r.t. model parameters p
ie	event index
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
ip	parameter index w.r.t. which the derivative is requested

Definition at line 1436 of file model.h.

10.11.3.154 fdrzdx() [2/2]

```
virtual void fdrzdx (
            realtype * drzdx,
            const int ie,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h )  [protected], [virtual]
```

model specific implementation of fdrzdx

Parameters

drzdx	partial derivative of root output rz w.r.t. model states x
ie	event index
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector

Definition at line 1449 of file model.h.

10.11.3.155 fdeltax() [2/2]

```
virtual void fdeltax (
            realtype * deltax,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ie,
```

```
            const realtype * xdot,
            const realtype * xdot_old )  [protected], [virtual]
```

model specific implementation of fdeltax

Parameters

deltax	state update
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
ie	event index
xdot	new model right hand side
xdot_old	previous model right hand side

Definition at line 1464 of file model.h.

10.11.3.156 fdeltasx() [2/2]

```
virtual void fdeltasx (
            realtype * deltasx,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * w,
            const int ip,
            const int ie,
            const realtype * xdot,
            const realtype * xdot_old,
            const realtype * sx,
            const realtype * stau )  [protected], [virtual]
```

model specific implementation of fdeltasx

Parameters

deltasx	sensitivity update
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
w	repeating elements vector
ip	sensitivity index
ie	event index
xdot	new model right hand side
xdot_old	previous model right hand side
sx	state sensitivity
stau	event-time sensitivity

Definition at line 1484 of file model.h.

10.11.3.157 fdeltaxB() [2/2]

```
virtual void fdeltaxB (
            realtype * deltaxB,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ie,
            const realtype * xdot,
            const realtype * xdot_old,
            const realtype * xB )  [protected], [virtual]
```

model specific implementation of fdeltaxB

Parameters

deltaxB	adjoint state update
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
ie	event index
xdot	new model right hand side
xdot_old	previous model right hand side
xB	current adjoint state

Definition at line 1502 of file model.h.

10.11.3.158 fdeltaqB() [2/2]

```
virtual void fdeltaqB (
            realtype * deltaqB,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ip,
            const int ie,
            const realtype * xdot,
            const realtype * xdot_old,
            const realtype * xB )  [protected], [virtual]
```

model specific implementation of fdeltaqB

Parameters

deltaqB	sensitivity update
t	current time
x	current state
p	parameter vector
k	constant vector
h	heavyside vector
ip	sensitivity index
ie	event index
xdot	new model right hand side
xdot_old	previous model right hand side
xB	adjoint state

Definition at line 1520 of file model.h.

10.11.3.159 fsigmay() [2/2]

```
virtual void fsigmay (
            realtype * sigmay,
            const realtype t,
            const realtype * p,
            const realtype * k )  [protected], [virtual]
```

model specific implementation of fsigmay

Parameters

sigmay	standard deviation of measurements
t	current time
p	parameter vector
k	constant vector

Definition at line 1531 of file model.h.

10.11.3.160 fdsigmaydp() [2/2]

```
virtual void fdsigmaydp (
            realtype * dsigmaydp,
            const realtype t,
            const realtype * p,
            const realtype * k,
            const int ip )  [protected], [virtual]
```

model specific implementation of fsigmay

Parameters

dsigmaydp	partial derivative of standard deviation of measurements
t	current time
p	parameter vector
k	constant vector
ip	sensitivity index

Definition at line 1542 of file model.h.

10.11.3.161 fsigmaz() [2/2]

```
virtual void fsigmaz (
            realtype * sigmaz,
            const realtype t,
            const realtype * p,
            const realtype * k )  [protected], [virtual]
```

model specific implementation of fsigmaz

Parameters

sigmaz	standard deviation of event measurements
t	current time
p	parameter vector
k	constant vector

Definition at line 1552 of file model.h.

10.11.3.162 fdsigmazdp() [2/2]

```
virtual void fdsigmazdp (
            realtype * dsigmazdp,
            const realtype t,
            const realtype * p,
            const realtype * k,
            const int ip )  [protected], [virtual]
```

model specific implementation of fsigmaz

Parameters

dsigmazdp	partial derivative of standard deviation of event measurements
t	current time
p	parameter vector
k	constant vector
ip	sensitivity index

Definition at line 1563 of file model.h.

10.11.3.163 fJy() [2/2]

```
virtual void fJy (
            realtype * nllh,
            const int iy,
            const realtype * p,
            const realtype * k,
            const realtype * y,
            const realtype * sigmay,
            const realtype * my )  [protected], [virtual]
```

model specific implementation of fJy

Parameters

nllh	negative log-likelihood for measurements y
iy	output index
p	parameter vector
k	constant vector
y	model output at timepoint
sigmay	measurement standard deviation at timepoint
my	measurements at timepoint

Definition at line 1576 of file model.h.

10.11.3.164 fJz() [2/2]

```
virtual void fJz (
            realtype * nllh,
            const int iz,
            const realtype * p,
            const realtype * k,
            const realtype * z,
            const realtype * sigmaz,
            const realtype * mz )  [protected], [virtual]
```

model specific implementation of fJz

Parameters

nllh	negative log-likelihood for event measurements z
iz	event output index
p	parameter vector
k	constant vector
z	model event output at timepoint
sigmaz	event measurement standard deviation at timepoint
mz	event measurements at timepoint

Definition at line 1588 of file model.h.

10.11.3.165 fJrz() [2/2]

```
virtual void fJrz (
            realtype * nllh,
            const int iz,
            const realtype * p,
            const realtype * k,
            const realtype * z,
            const realtype * sigmaz )  [protected], [virtual]
```

model specific implementation of fJrz

Parameters

nllh	regularization for event measurements z
iz	event output index
p	parameter vector
k	constant vector
z	model event output at timepoint
sigmaz	event measurement standard deviation at timepoint

Definition at line 1600 of file model.h.

10.11.3.166 fdJydy() [2/2]

```
virtual void fdJydy (
            realtype * dJydy,
            const int iy,
            const realtype * p,
            const realtype * k,
            const realtype * y,
            const realtype * sigmay,
            const realtype * my )  [protected], [virtual]
```

model specific implementation of fdJydy

Parameters

dJydy	partial derivative of time-resolved measurement negative log-likelihood Jy
iy	output index
p	parameter vector
k	constant vector
y	model output at timepoint
sigmay	measurement standard deviation at timepoint
my	measurement at timepoint

Definition at line 1613 of file model.h.

10.11.3.167 fdJydsigma() [2/2]

```
virtual void fdJydsigma (
            realtype * dJydsigma,
            const int iy,
            const realtype * p,
            const realtype * k,
            const realtype * y,
            const realtype * sigmay,
            const realtype * my )  [protected], [virtual]
```

model specific implementation of fdJydsigma

Parameters

dJydsigma	Sensitivity of time-resolved measurement negative log-likelihood Jy w.r.t. standard deviation sigmay
iy	output index
p	parameter vector
k	constant vector
y	model output at timepoint
sigmay	measurement standard deviation at timepoint
my	measurement at timepoint

Definition at line 1628 of file model.h.

10.11.3.168 fdJzdz() [2/2]

```
virtual void fdJzdz (
            realtype * dJzdz,
            const int iz,
            const realtype * p,
            const realtype * k,
            const realtype * z,
            const realtype * sigmaz,
            const realtype * mz )  [protected], [virtual]
```

model specific implementation of fdJzdz

Parameters

dJzdz	partial derivative of event measurement negative log-likelihood Jz
iz	event output index
p	parameter vector
k	constant vector
z	model event output at timepoint
sigmaz	event measurement standard deviation at timepoint
mz	event measurement at timepoint

Definition at line 1642 of file model.h.

10.11.3.169 fdJzdsigma() [2/2]

```
virtual void fdJzdsigma (
            realtype * dJzdsigma,
            const int iz,
            const realtype * p,
            const realtype * k,
            const realtype * z,
            const realtype * sigmaz,
            const realtype * mz )  [protected], [virtual]
```

model specific implementation of fdJzdsigma

Parameters

dJzdsigma	Sensitivity of event measurement negative log-likelihood Jz w.r.t. standard deviation sigmaz
iz	event output index
p	parameter vector
k	constant vector
z	model event output at timepoint
sigmaz	event measurement standard deviation at timepoint
mz	event measurement at timepoint

Definition at line 1657 of file model.h.

10.11.3.170 fdJrzdz() [2/2]

```
virtual void fdJrzdz (
            realtype * dJrzdz,
            const int iz,
            const realtype * p,
            const realtype * k,
            const realtype * rz,
            const realtype * sigmaz )  [protected], [virtual]
```

model specific implementation of fdJrzdz

Parameters

dJrzdz	partial derivative of event penalization Jrz
iz	event output index
p	parameter vector
k	constant vector
rz	model root output at timepoint
sigmaz	event measurement standard deviation at timepoint

Definition at line 1670 of file model.h.

10.11.3.171 fdJrzdsigma() [2/2]

```
virtual void fdJrzdsigma (
            realtype * dJrzdsigma,
            const int iz,
            const realtype * p,
            const realtype * k,
            const realtype * rz,
            const realtype * sigmaz )  [protected], [virtual]
```

model specific implementation of fdJrzdsigma

Parameters

dJrzdsigma	Sensitivity of event penalization Jrz w.r.t. standard deviation sigmaz
iz	event output index
p	parameter vector
k	constant vector
rz	model root output at timepoint
sigmaz	event measurement standard deviation at timepoint

Definition at line 1684 of file model.h.

10.11.3.172 fw() [2/2]

```
virtual void fw (
            realtype * w,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * tcl )  [protected], [virtual]
```

model specific implementation of fw

Parameters

w	Recurring terms in xdot
t	timepoint
x	vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
tcl	total abundances for conservations laws

Definition at line 1698 of file model.h.

10.11.3.173 fdwdp() [2/2]

```
virtual void fdwdp (
            realtype * dwdp,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * w,
            const realtype * tcl,
            const realtype * stcl )  [protected], [virtual]
```

model specific implementation of dwdp

Parameters

dwdp	Recurring terms in xdot, parameter derivative
t	timepoint
x	vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
w	vector with helper variables
tcl	total abundances for conservations laws
stcl	sensitivities of total abundances for conservations laws

Definition at line 1712 of file model.h.

10.11.3.174 fdwdx() [2/2]

```
virtual void fdwdx (
            realtype * dwdx,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * w,
            const realtype * tcl )  [protected], [virtual]
```

model specific implementation of dwdx

Parameters

dwdx	Recurring terms in xdot, state derivative
t	timepoint
x	vector with the states

Parameters

p	parameter vector
k	constants vector
h	heavyside vector
w	vector with helper variables
tcl	total abundances for conservations laws

Definition at line 1726 of file model.h.

10.11.3.175 getmy()

```
void getmy (
            const int it,
            const ExpData * edata )  [protected]
```

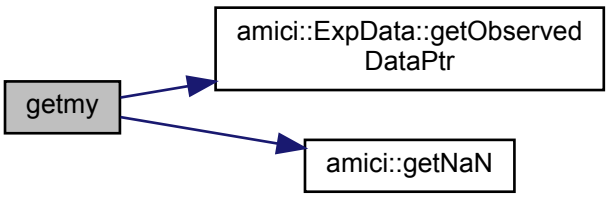
create my slice at timepoint

Parameters

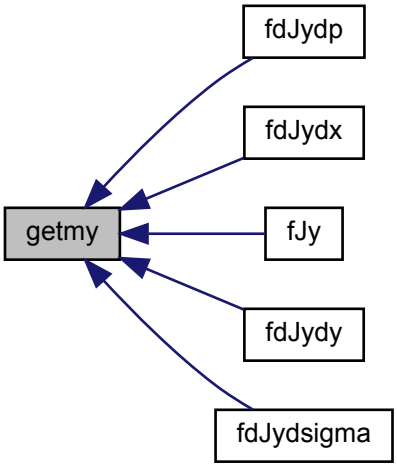
it	timepoint index
edata	pointer to experimental data instance

Definition at line 1292 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.176 getmz()

```
void getmz (
            const int nroots,
            const ExpData * edata )  [protected]
```

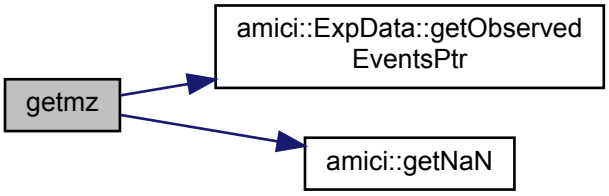
create mz slice at event

Parameters

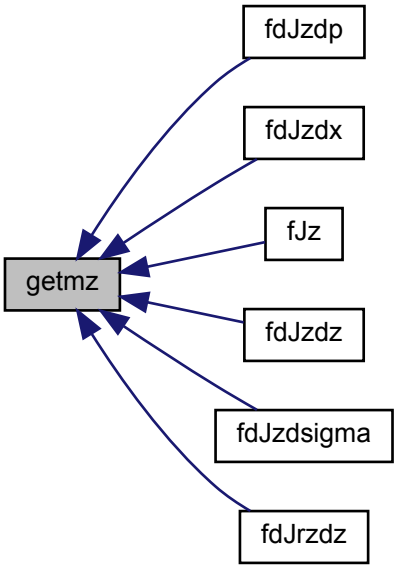
nroots	event occurence
edata	pointer to experimental data instance

Definition at line 1308 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.3.177 gety()

```
const realtype * gety (
            const int it,
            const ReturnData * rdata ) const  [protected]
```

create y slice at timepoint

Parameters

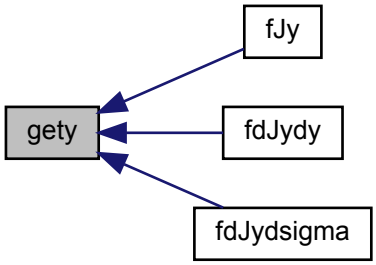
it	timepoint index
rdata	pointer to return data instance

Returns

y y-slice from rdata instance

Definition at line 1300 of file model.cpp.

Here is the caller graph for this function:



10.11.3.178 getz()

```
const realtype * getz (
            const int nroots,
            const ReturnData * rdata ) const  [protected]
```

create z slice at event

Parameters

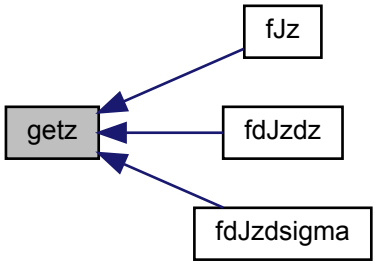
nroots	event occurence
rdata	pointer to return data instance

Returns

z slice

Definition at line 1316 of file model.cpp.

Here is the caller graph for this function:



10.11.3.179 getrz()

```
const realtype * getrz (
            const int nroots,
            const ReturnData * rdata ) const  [protected]
```

create rz slice at event

Parameters

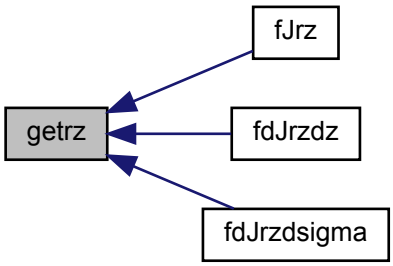
nroots	event occurence
rdata	pointer to return data instance

Returns

rz slice

Definition at line 1320 of file model.cpp.

Here is the caller graph for this function:



10.11.3.180 getsz()

```
const realtype * getsz (
            const int nroots,
            const int ip,
            const ReturnData * rdata ) const  [protected]
```

create sz slice at event

Parameters

nroots	event occurence
ip	sensitivity index
rdata	pointer to return data instance

Returns

z slice

Definition at line 1324 of file model.cpp.

Here is the call graph for this function:

10.11.3.181 getsrz()

```
const realtype * getsrz (
            const int nroots,
            const int ip,
            const ReturnData * rdata ) const  [protected]
```

create srz slice at event

Parameters

nroots	event occurence
ip	sensitivity index
rdata	pointer to return data instance

Returns

rz slice

Definition at line 1328 of file model.cpp.

Here is the call graph for this function:

10.11.3.182 isFixedParameterStateReinitializationAllowed()

```
virtual bool isFixedParameterStateReinitializationAllowed ( ) const  [protected], [virtual]
```

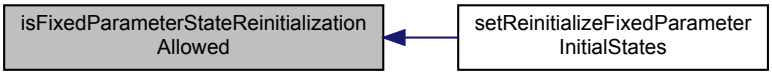
function indicating whether reinitialization of states depending on fixed parameters is permissible

Returns

flag inidication whether reinitialization of states depending on fixed parameters is permissible

Definition at line 1783 of file model.h.

Here is the caller graph for this function:



10.11.3.183 computeX_pos()

```
N_Vector computeX_pos (
            N_Vector x )  [protected]
```

Parameters

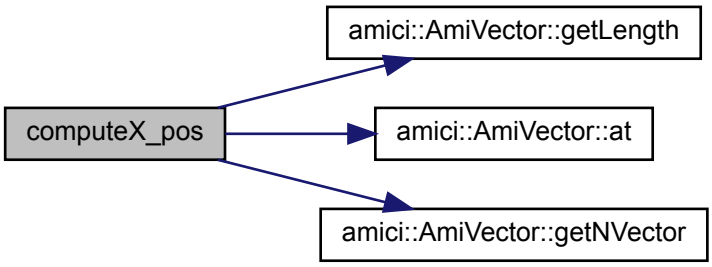
x	state vector possibly containing negative values

Returns

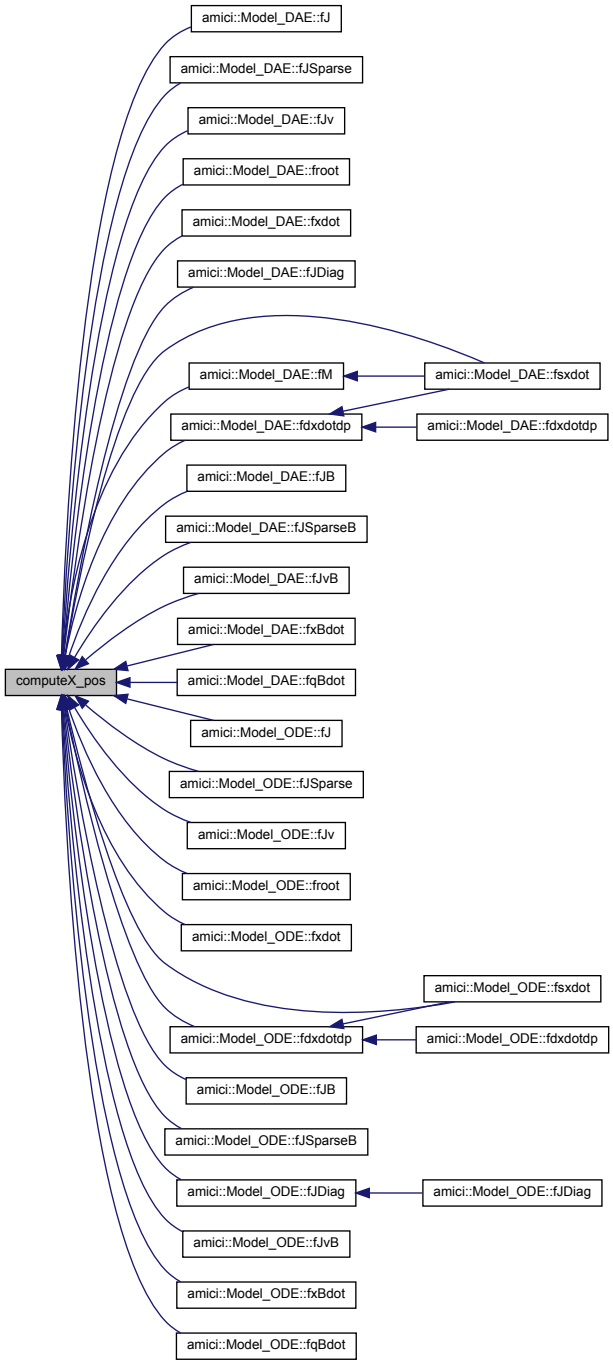
state vector with negative values replaced by 0 according to stateIsNonNegative

Definition at line 1390 of file model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.11.4 Friends And Related Function Documentation

10.11.4.1 boost::serialization::serialize

```
void boost::serialization::serialize (
            Archive & ar,
```

```
            Model & r,
            const unsigned int version )  [friend]
```

Parameters

ar	Archive to serialize to
r	Data to serialize
version	Version number

10.11.4.2 operator==

```
bool operator== (
            const Model & a,
            const Model & b )  [friend]
```

Parameters

a	first model instance
b	second model instance

Returns

equality

Definition at line 1352 of file model.cpp.

10.11.5 Member Data Documentation

10.11.5.1 nx_rdata

```
const int nx_rdata
```

number of states

Definition at line 1095 of file model.h.

10.11.5.2 nxtrue_rdata

```
const int nxtrue_rdata
```

number of states in the unaugmented system

Definition at line 1097 of file model.h.

10.11.5.3 nx_solver

```
const int nx_solver
```

number of states with conservation laws applied

Definition at line 1099 of file model.h.

10.11.5.4 nxtrue_solver

```
const int nxtrue_solver
```

number of states in the unaugmented system with conservation laws applied

Definition at line 1101 of file model.h.

10.11.5.5 ny

```
const int ny
```

number of observables

Definition at line 1103 of file model.h.

10.11.5.6 nytrue

```
const int nytrue
```

number of observables in the unaugmented system

Definition at line 1105 of file model.h.

10.11.5.7 nz

```
const int nz
```

number of event outputs

Definition at line 1107 of file model.h.

10.11.5.8 nztrue

```
const int nztrue
```

number of event outputs in the unaugmented system

Definition at line 1109 of file model.h.

10.11.5.9 ne

```
const int ne
```

number of events

Definition at line 1111 of file model.h.

10.11.5.10 nw

```
const int nw
```

number of common expressions

Definition at line 1113 of file model.h.

10.11.5.11 ndwdx

```
const int ndwdx
```

number of derivatives of common expressions wrt x

Definition at line 1115 of file model.h.

10.11.5.12 ndwdp

```
const int ndwdp
```

number of derivatives of common expressions wrt p

Definition at line 1117 of file model.h.

10.11.5.13 nnz

```
const int nnz
```

number of nonzero entries in jacobian

Definition at line 1119 of file model.h.

10.11.5.14 nJ

```
const int nJ
```

dimension of the augmented objective function for 2nd order ASA

Definition at line 1121 of file model.h.

10.11.5.15 ubw

```
const int ubw
```

upper bandwith of the jacobian

Definition at line 1123 of file model.h.

10.11.5.16 lbw

```
const int lbw
```

lower bandwith of the jacobian

Definition at line 1125 of file model.h.

10.11.5.17 o2mode

```
const SecondOrderMode o2mode
```

flag indicating whether for sensi == AMICI_SENSI_ORDER_SECOND directional or full second order derivative will be computed

Definition at line 1128 of file model.h.

10.11.5.18 z2event

```
const std::vector<int> z2event
```

index indicating to which event an event output belongs

Definition at line 1130 of file model.h.

10.11.5.19 idlist

```
const std::vector<realtype> idlist
```

flag array for DAE equations

Definition at line 1132 of file model.h.

10.11.5.20 sigmay

```
std::vector<realtype> sigmay
```

data standard deviation for current timepoint (dimension: ny)

Definition at line 1135 of file model.h.

10.11.5.21 dsigmaydp

```
std::vector<realtype> dsigmaydp
```

parameter derivative of data standard deviation for current timepoint (dimension: nplist x ny, row-major)

Definition at line 1137 of file model.h.

10.11.5.22 sigmaz

```
std::vector<realtype> sigmaz
```

event standard deviation for current timepoint (dimension: nz)

Definition at line 1139 of file model.h.

10.11.5.23 dsigmazdp

```
std::vector<realtype> dsigmazdp
```

parameter derivative of event standard deviation for current timepoint (dimension: nplist x nz, row-major)

Definition at line 1141 of file model.h.

10.11.5.24 dJydp

```
std::vector<realtype> dJydp
```

parameter derivative of data likelihood for current timepoint (dimension: nplist x nJ, row-major)

Definition at line 1143 of file model.h.

10.11.5.25 dJzdp

```
std::vector<realtype> dJzdp
```

parameter derivative of event likelihood for current timepoint (dimension: nplist x nJ, row-major)

Definition at line 1145 of file model.h.

10.11.5.26 deltax

```
std::vector<realtype> deltax
```

change in x at current timepoint (dimension: nx_solver)

Definition at line 1148 of file model.h.

10.11.5.27 deltasx

```
std::vector<realtype> deltasx
```

change in sx at current timepoint (dimension: nplist x nx_solver, row-major)

Definition at line 1150 of file model.h.

10.11.5.28 deltaxB

```
std::vector<realtype> deltaxB
```

change in xB at current timepoint (dimension: nJ x nxtrue_cl, row-major)

Definition at line 1152 of file model.h.

10.11.5.29 deltaqB

```
std::vector<realtype> deltaqB
```

change in qB at current timepoint (dimension: nJ x nplist, row-major)

Definition at line 1154 of file model.h.

10.11.5.30 dxdotdp

```
std::vector<realtype> dxdotdp
```

tempory storage of dxdotdp data across functions (dimension: nplist x nx_solver, row-major)

Definition at line 1157 of file model.h.

10.11.5.31 J

```
SlsMat J = nullptr  [protected]
```

Sparse Jacobian (dimension: nnz)

Definition at line 1789 of file model.h.

10.11.5.32 my

```
std::vector<realtype> my  [protected]
```

current observable (dimension: nytrue)

Definition at line 1792 of file model.h.

10.11.5.33 mz

```
std::vector<realtype> mz  [protected]
```

current event measurement (dimension: nztrue)

Definition at line 1794 of file model.h.

10.11.5.34 dJydy

```
std::vector<realtype> dJydy  [protected]
```

observable derivative of data likelihood (dimension nJ x nytrue x ny, ordering = ?)

Definition at line 1796 of file model.h.

10.11.5.35 dJydsigma

```
std::vector<realtype> dJydsigma  [protected]
```

observable sigma derivative of data likelihood (dimension nJ x nytrue x ny, ordering = ?)

Definition at line 1798 of file model.h.

10.11.5.36 dJzdz

```
std::vector<realtype> dJzdz  [protected]
```

event ouput derivative of event likelihood (dimension nJ x nztrue x nz, ordering = ?)

Definition at line 1801 of file model.h.

10.11.5.37 dJzdsigma

```
std::vector<realtype> dJzdsigma  [protected]
```

event sigma derivative of event likelihood (dimension nJ x nztrue x nz, ordering = ?)

Definition at line 1803 of file model.h.

10.11.5.38 dJrzdz

```
std::vector<realtype> dJrzdz [protected]
```

event ouput derivative of event likelihood at final timepoint (dimension nJ x nztrue x nz, ordering = ?)

Definition at line 1805 of file model.h.

10.11.5.39 dJrzdsigma

```
std::vector<realtype> dJrzdsigma [protected]
```

event sigma derivative of event likelihood at final timepoint (dimension nJ x nztrue x nz, ordering = ?)

Definition at line 1807 of file model.h.

10.11.5.40 dzdx

```
std::vector<realtype> dzdx [protected]
```

state derivative of event output (dimension: nz x nx_solver, ordering = ?)

Definition at line 1809 of file model.h.

10.11.5.41 dzdp

```
std::vector<realtype> dzdp [protected]
```

parameter derivative of event output (dimension: nz x nplist, ordering = ?)

Definition at line 1811 of file model.h.

10.11.5.42 drzdx

```
std::vector<realtype> drzdx [protected]
```

state derivative of event timepoint (dimension: nz x nx_solver, ordering = ?)

Definition at line 1813 of file model.h.

10.11.5.43 drzdp

```
std::vector<realtype> drzdp  [protected]
```

parameter derivative of event timepoint (dimension: nz x nplist, ordering = ?)

Definition at line 1815 of file model.h.

10.11.5.44 dydp

```
std::vector<realtype> dydp  [protected]
```

parameter derivative of observable (dimension: nplist x ny, row-major)

Definition at line 1817 of file model.h.

10.11.5.45 dydx

```
std::vector<realtype> dydx  [protected]
```

state derivative of observable (dimension: ny x nx_solver, ordering = ?)

Definition at line 1820 of file model.h.

10.11.5.46 w

```
std::vector<realtype> w  [protected]
```

tempory storage of w data across functions (dimension: nw)

Definition at line 1822 of file model.h.

10.11.5.47 dwdx

```
std::vector<realtype> dwdx  [protected]
```

tempory storage of sparse dwdx data across functions (dimension: ndwdx)

Definition at line 1824 of file model.h.

10.11.5.48 dwdp

```
std::vector<realtype> dwdp [protected]
```

tempory storage of sparse dwdp data across functions (dimension: ndwdp)

Definition at line 1826 of file model.h.

10.11.5.49 M

```
std::vector<realtype> M [protected]
```

tempory storage of mass matrix data across functions (dimension: nx_solver)

Definition at line 1828 of file model.h.

10.11.5.50 stau

```
std::vector<realtype> stau [protected]
```

tempory storage of stau data across functions (dimension: nplist)

Definition at line 1830 of file model.h.

10.11.5.51 sx

```
std::vector<realtype> sx [protected]
```

tempory storage of sx data for flattening (dimension: nx_solver x nplist, ordering = ?)

Definition at line 1833 of file model.h.

10.11.5.52 x_rdata

```
std::vector<realtype> x_rdata [protected]
```

tempory storage x_rdata (dimension: nx_rdata)

Definition at line 1836 of file model.h.

10.11.5.53 sx_rdata

```
std::vector<realtype> sx_rdata [protected]
```

tempory storage sx_rdata slice (dimension: nx_rdata)

Definition at line 1838 of file model.h.

10.11.5.54 h

```
std::vector<realtype> h [protected]
```

flag indicating whether a certain heaviside function should be active or not (dimension: ne)

Definition at line 1842 of file model.h.

10.11.5.55 unscaledParameters

```
std::vector<realtype> unscaledParameters [protected]
```

unscaled parameters (dimension: np)

Definition at line 1845 of file model.h.

10.11.5.56 originalParameters

```
std::vector<realtype> originalParameters [protected]
```

orignal user-provided, possibly scaled parameter array (size np)

Definition at line 1848 of file model.h.

10.11.5.57 fixedParameters

```
std::vector<realtype> fixedParameters [protected]
```

constants (dimension: nk)

Definition at line 1851 of file model.h.

10.11.5.58 total_cl

```
std::vector<realtype> total_cl [protected]
```

total abundances for conservation laws (dimension: nx_rdata-nx_solver)

Definition at line 1854 of file model.h.

10.11.5.59 stotal_cl

```
std::vector<realtype> stotal_cl [protected]
```

sensitivities of total abundances for conservation laws (dimension: nx_rdata-nx_solver x nplist)

Definition at line 1857 of file model.h.

10.11.5.60 plist_

```
std::vector<int> plist_ [protected]
```

indexes of parameters wrt to which sensitivities are computed (dimension nplist)

Definition at line 1860 of file model.h.

10.11.5.61 x0data

```
std::vector<double> x0data [protected]
```

state initialisation (size nx_solver)

Definition at line 1863 of file model.h.

10.11.5.62 sx0data

```
std::vector<realtype> sx0data [protected]
```

sensitivity initialisation (size nx_solver $*$ nplist, ordering = ?)

Definition at line 1866 of file model.h.

10.11.5.63 ts

```
std::vector<realtype> ts  [protected]
```

timepoints (size nt)

Definition at line 1869 of file model.h.

10.11.5.64 stateIsNonNegative

```
std::vector<bool> stateIsNonNegative  [protected]
```

vector of bools indicating whether state variables are to be assumed to be positive

Definition at line 1872 of file model.h.

10.11.5.65 anyStateNonNegative

```
bool anyStateNonNegative = false  [protected]
```

boolean indicating whether any entry in stateIsNonNegative is `true`

Definition at line 1875 of file model.h.

10.11.5.66 x_pos_tmp

```
AmiVector x_pos_tmp  [protected]
```

temporary storage of positified state variables according to stateIsNonNegative

Definition at line 1878 of file model.h.

10.11.5.67 nmaxevent

```
int nmaxevent = 10  [protected]
```

maximal number of events to track

Definition at line 1881 of file model.h.

10.11.5.68 pscale

```
std::vector<ParameterScaling> pscale  [protected]
```

parameter transformation of `originalParameters` (dimension np)

Definition at line 1884 of file model.h.

10.11.5.69 tstart

```
double tstart = 0.0  [protected]
```

starting time

Definition at line 1887 of file model.h.

10.11.5.70 steadyStateSensitivityMode

```
SteadyStateSensitivityMode steadyStateSensitivityMode = SteadyStateSensitivityMode::newtonOnly
[protected]
```

flag indicating whether steadystate sensivities are to be computed via FSA when steadyStateSimulation is used

Definition at line 1891 of file model.h.

10.11.5.71 reinitializeFixedParameterInitialStates

```
bool reinitializeFixedParameterInitialStates = false  [protected]
```

flag indicating whether reinitialization of states depending on fixed parameters is activated

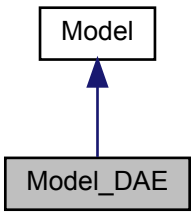
Definition at line 1896 of file model.h.

10.12 Model_DAE Class Reference

The Model class represents an AMICI DAE model. The model does not contain any data, but represents the state of the model at a specific time t. The states must not always be in sync, but may be updated asynchroneously.

```
#include <model_dae.h>
```

Inheritance diagram for Model_DAE:



Public Member Functions

- Model_DAE ()
- Model_DAE (const int nx_rdata, const int nxtrue_rdata, const int nx_solver, const int nxtrue_solver, const int ny, const int nytrue, const int nz, const int nztrue, const int ne, const int nJ, const int nw, const int ndwdx, const int ndwdp, const int nnz, const int ubw, const int lbw, const SecondOrderMode o2mode, const std::vector< realtype > p, const std::vector< realtype > k, const std::vector< int > plist, const std::vector< realtype > idlist, const std::vector< int > z2event)
- virtual void fJ (realtype t, realtype cj, AmiVector *x, AmiVector *dx, AmiVector *xdot, DlsMat J) override
- void fJ (realtype t, realtype cj, N_Vector x, N_Vector dx, N_Vector xdot, DlsMat J)
- void fJB (realtype t, realtype cj, N_Vector x, N_Vector dx, N_Vector xB, N_Vector dxB, DlsMat JB)
- virtual void fJSparse (realtype t, realtype cj, AmiVector *x, AmiVector *dx, AmiVector *xdot, SlsMat J) override
- void fJSparse (realtype t, realtype cj, N_Vector x, N_Vector dx, SlsMat J)
- void fJSparseB (realtype t, realtype cj, N_Vector x, N_Vector dx, N_Vector xB, N_Vector dxB, SlsMat JB)
- virtual void fJDiag (realtype t, AmiVector *JDiag, realtype cj, AmiVector *x, AmiVector *dx) override
- virtual void fJv (realtype t, AmiVector *x, AmiVector *dx, AmiVector *xdot, AmiVector *v, AmiVector *nJv, realtype cj) override
- void fJv (realtype t, N_Vector x, N_Vector dx, N_Vector v, N_Vector Jv, realtype cj)
- void fJvB (realtype t, N_Vector x, N_Vector dx, N_Vector xB, N_Vector dxB, N_Vector vB, N_Vector JvB, realtype cj)
- virtual void froot (realtype t, AmiVector *x, AmiVector *dx, realtype *root) override
- void froot (realtype t, N_Vector x, N_Vector dx, realtype *root)
- virtual void fxdot (realtype t, AmiVector *x, AmiVector *dx, AmiVector *xdot) override
- void fxdot (realtype t, N_Vector x, N_Vector dx, N_Vector xdot)
- void fxBdot (realtype t, N_Vector x, N_Vector dx, N_Vector xB, N_Vector dxB, N_Vector xBdot)
- void fqBdot (realtype t, N_Vector x, N_Vector dx, N_Vector xB, N_Vector dxB, N_Vector qBdot)
- void fdxdotdp (const realtype t, const N_Vector x, const N_Vector dx)
- virtual void fdxdotdp (realtype t, AmiVector *x, AmiVector *dx) override
- void fsxdot (realtype t, AmiVector *x, AmiVector *dx, int ip, AmiVector *sx, AmiVector *sdx, AmiVector *sxdot) override
- void fsxdot (realtype t, N_Vector x, N_Vector dx, int ip, N_Vector sx, N_Vector sdx, N_Vector sxdot)
- void fM (realtype t, const N_Vector x)

  Mass matrix for DAE systems.
- virtual std::unique_ptr< Solver > getSolver () override

Protected Member Functions

- virtual void fJ (realtype *J, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype cj, const realtype *dx, const realtype *w, const realtype *dwdx)=0
- virtual void fJB (realtype *JB, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype cj, const realtype *xB, const realtype *dx, const realtype *dxB, const realtype *w, const realtype *dwdx)
- virtual void fJSparse (SlsMat JSparse, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype cj, const realtype *dx, const realtype *w, const realtype *dwdx)=0
- virtual void fJSparseB (SlsMat JSparseB, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype cj, const realtype *xB, const realtype *dx, const realtype *dxB, const realtype *w, const realtype *dwdx)
- virtual void fJDiag (realtype *JDiag, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype cj, const realtype *dx, const realtype *w, const realtype *dwdx)
- virtual void fJv (realtype *Jv, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype cj, const realtype *dx, const realtype *v, const realtype *w, const realtype *dwdx)
- virtual void fJvB (realtype *JvB, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype cj, const realtype *xB, const realtype *dx, const realtype *dxB, const realtype *vB, const realtype *w, const realtype *dwdx)

- virtual void froot (realtype *root, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype *dx)
- virtual void fxdot (realtype *xdot, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype *dx, const realtype *w)=0
- virtual void fxBdot (realtype *xBdot, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype *xB, const realtype *dx, const realtype *dxB, const realtype *w, const realtype *dwdx)
- virtual void fqBdot (realtype *qBdot, const int ip, const realtype t, const realtype *x, const double *p, const double *k, const realtype *h, const realtype *xB, const realtype *dx, const realtype *dxB, const realtype *w, const realtype *dwdp)
- virtual void fdxdotdp (realtype *dxdotdp, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const int ip, const realtype *dx, const realtype *w, const realtype *dwdp)
- virtual void fsxdot (realtype *sxdot, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const int ip, const realtype *dx, const realtype *sx, const realtype *sdx, const realtype *w, const realtype *dwdx, const realtype *M, const realtype *J, const realtype *dxdotdp)
- virtual void fM (realtype *M, const realtype t, const realtype *x, const realtype *p, const realtype *k)

Additional Inherited Members

10.12.1 Detailed Description

Definition at line 24 of file model_dae.h.

10.12.2 Constructor & Destructor Documentation

10.12.2.1 Model_DAE() [1/2]

```
Model_DAE ( )
```

default constructor

Definition at line 27 of file model_dae.h.

10.12.2.2 Model_DAE() [2/2]

```
Model_DAE (
            const int nx_rdata,
            const int nxtrue_rdata,
            const int nx_solver,
            const int nxtrue_solver,
            const int ny,
            const int nytrue,
            const int nz,
            const int nztrue,
            const int ne,
            const int nJ,
            const int nw,
            const int ndwdx,
            const int ndwdp,
```

```
            const int nnz,
            const int ubw,
            const int lbw,
            const SecondOrderMode o2mode,
            const std::vector< realtype > p,
            const std::vector< realtype > k,
            const std::vector< int > plist,
            const std::vector< realtype > idlist,
            const std::vector< int > z2event )
```

constructor with model dimensions

Parameters

nx_rdata	number of state variables
nxtrue_rdata	number of state variables of the non-augmented model
nx_solver	number of state variables with conservation laws applied
nxtrue_solver	number of state variables of the non-augmented model with conservation laws applied
ny	number of observables
nytrue	number of observables of the non-augmented model
nz	number of event observables
nztrue	number of event observables of the non-augmented model
ne	number of events
nJ	number of objective functions
nw	number of repeating elements
ndwdx	number of nonzero elements in the x derivative of the repeating elements
ndwdp	number of nonzero elements in the p derivative of the repeating elements
nnz	number of nonzero elements in Jacobian
ubw	upper matrix bandwidth in the Jacobian
lbw	lower matrix bandwidth in the Jacobian
o2mode	second order sensitivity mode
p	parameters
k	constants
plist	indexes wrt to which sensitivities are to be computed
idlist	indexes indicating algebraic components (DAE only)
z2event	mapping of event outputs to events

Definition at line 56 of file model_dae.h.

10.12.3 Member Function Documentation

10.12.3.1 fJ() [1/3]

```
void fJ (
            realtype t,
            realtype cj,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot,
            DlsMat J )  [override], [virtual]
```

Dense Jacobian function

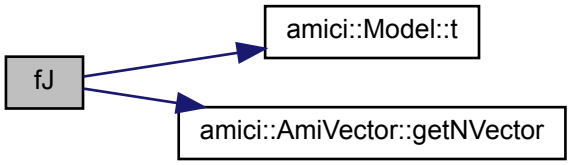
Parameters

t	time
cj	scaling factor (inverse of timestep, DAE only)
x	state
dx	time derivative of state (DAE only)
xdot	values of residual function (unused)
J	dense matrix to which values of the jacobian will be written

Implements Model.

Definition at line 6 of file model_dae.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.12.3.2 fJ() [2/3]

```
void fJ (
            realtype t,
            realtype cj,
            N_Vector x,
            N_Vector dx,
            N_Vector xdot,
            DlsMat J )
```

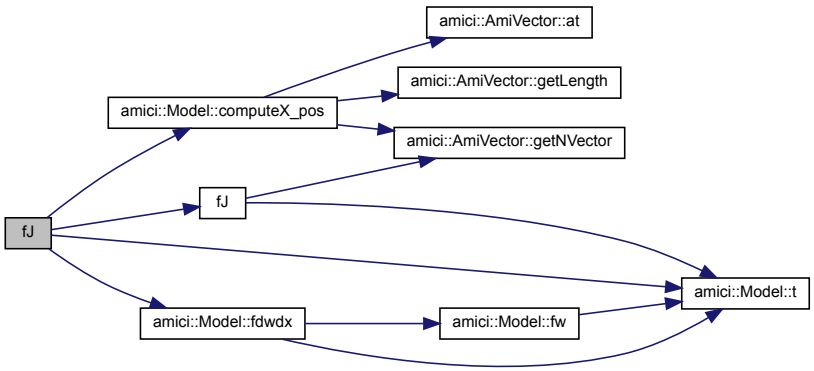
Jacobian of xdot with respect to states x

Parameters

t	timepoint
cj	scaling factor, inverse of the step size
x	Vector with the states
dx	Vector with the derivative states
xdot	Vector with the right hand side
J	Matrix to which the Jacobian will be written

Definition at line 20 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.3 fJB() [1/2]

```
void fJB (
            realtype t,
            realtype cj,
            N_Vector x,
            N_Vector dx,
            N_Vector xB,
            N_Vector dxB,
            DlsMat JB )
```

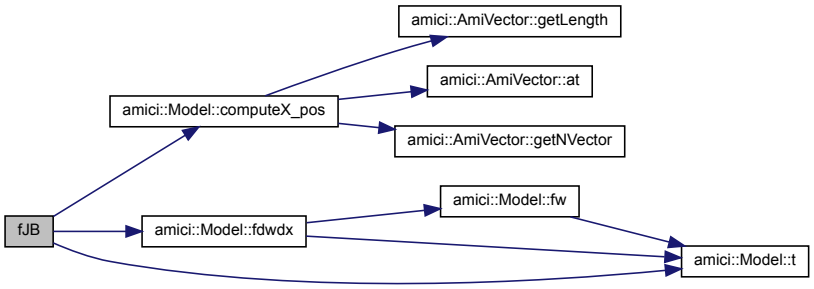
Jacobian of xBdot with respect to adjoint state xB

Parameters

t	timepoint
cj	scaling factor, inverse of the step size
x	Vector with the states
dx	Vector with the derivative states
xB	Vector with the adjoint states
dxB	Vector with the adjoint derivative states
JB	Matrix to which the Jacobian will be written

Definition at line 166 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.4 fJSparse() [1/3]

```
void fJSparse (
            realtype t,
            realtype cj,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot,
            SlsMat J )  [override], [virtual]
```

Sparse Jacobian function

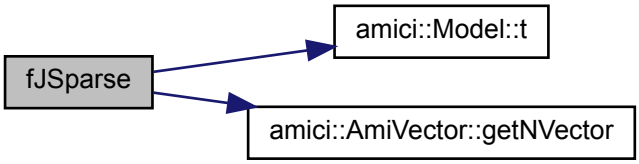
Parameters

t	time
cj	scaling factor (inverse of timestep, DAE only)
x	state
dx	time derivative of state (DAE only)
xdot	values of residual function (unused)
J	sparse matrix to which values of the Jacobian will be written

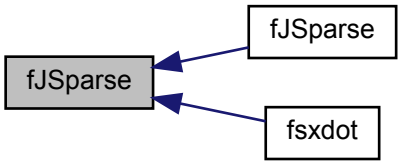
Implements Model.

Definition at line 29 of file model_dae.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.12.3.5 fJSparse() [2/3]

```
void fJSparse (
            realtype t,
            realtype cj,
            N_Vector x,
            N_Vector dx,
            SlsMat J )
```

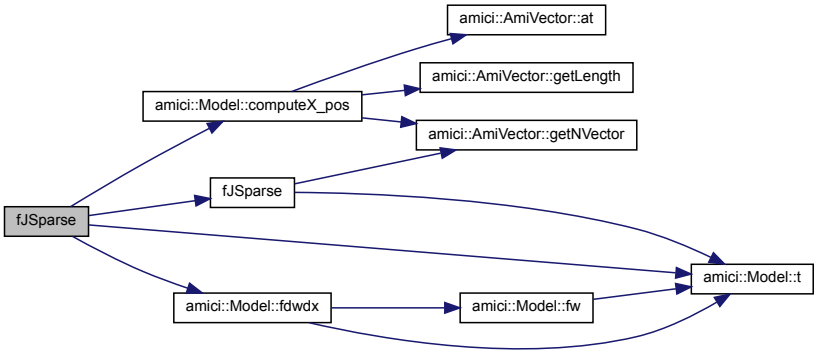
J in sparse form (for sparse solvers from the SuiteSparse Package)

Parameters

t	timepoint
cj	scalar in Jacobian (inverse stepsize)
x	Vector with the states
dx	Vector with the derivative states
J	Matrix to which the Jacobian will be written

Definition at line 41 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.6 fJSparseB() [1/2]

```
void fJSparseB (
            realtype t,
            realtype cj,
            N_Vector x,
            N_Vector dx,
            N_Vector xB,
            N_Vector dxB,
            SlsMat JB )
```

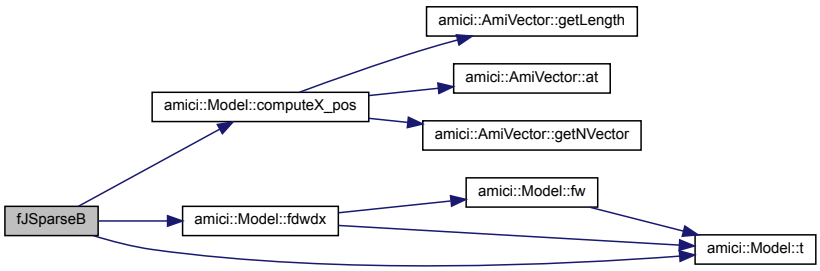
JB in sparse form (for sparse solvers from the SuiteSparse Package)

Parameters

t	timepoint
cj	scalar in Jacobian
x	Vector with the states
dx	Vector with the derivative states
xB	Vector with the adjoint states
dxB	Vector with the adjoint derivative states
JB	Matrix to which the Jacobian will be written

Definition at line 184 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.7 fJDiag() [1/2]

```
void fJDiag (
            realtype t,
            AmiVector * JDiag,
            realtype cj,
            AmiVector * x,
            AmiVector * dx )  [override], [virtual]
```

diagonalized Jacobian (for preconditioning)

Parameters

t	timepoint
JDiag	Vector to which the Jacobian diagonal will be written
cj	scaling factor, inverse of the step size
x	Vector with the states
dx	Vector with the derivative states

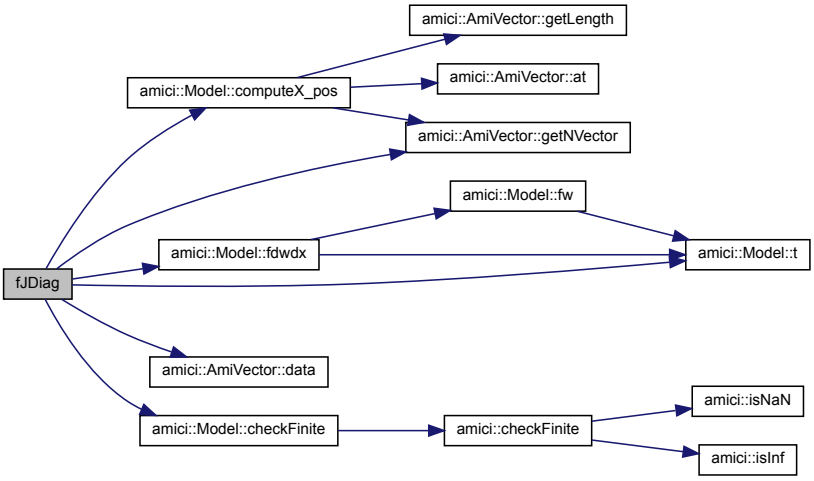
Returns

status flag indicating successful execution

Implements Model.

Definition at line 116 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.8 fJv() [1/3]

```
void fJv (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot,
            AmiVector * v,
            AmiVector * nJv,
            realtype cj )  [override], [virtual]
```

Jacobian multiply function

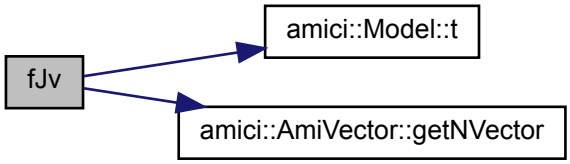
Parameters

t	time
x	state
dx	time derivative of state (DAE only)
xdot	values of residual function (unused)
v	multiplication vector (unused)
nJv	array to which result of multiplication will be written
cj	scaling factor (inverse of timestep, DAE only)

Implements Model.

Definition at line 49 of file model_dae.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.12.3.9 fJv() [2/3]

```
void fJv (
            realtype t,
            N_Vector x,
            N_Vector dx,
            N_Vector v,
            N_Vector Jv,
            realtype cj )
```

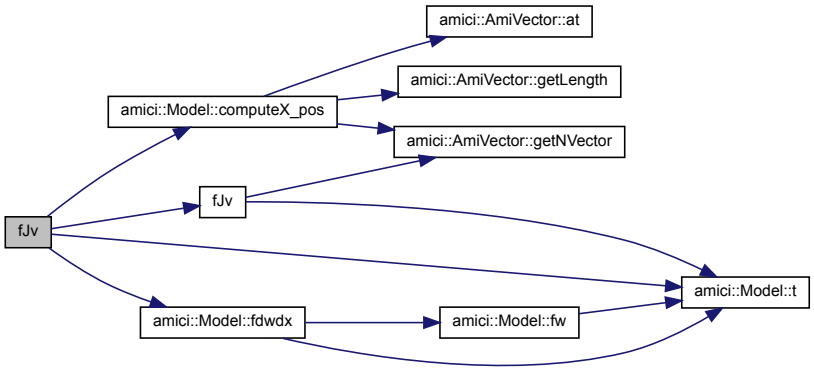
Matrix vector product of J with a vector v (for iterative solvers)

Parameters

t	timepoint **Type**: realtype
cj	scaling factor, inverse of the step size
x	Vector with the states
dx	Vector with the derivative states
v	Vector with which the Jacobian is multiplied
Jv	Vector to which the Jacobian vector product will be written

Definition at line 64 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.10 fJvB() [1/2]

```
void fJvB (
            realtype t,
            N_Vector x,
            N_Vector dx,
            N_Vector xB,
            N_Vector dxB,
            N_Vector vB,
            N_Vector JvB,
            realtype cj )
```

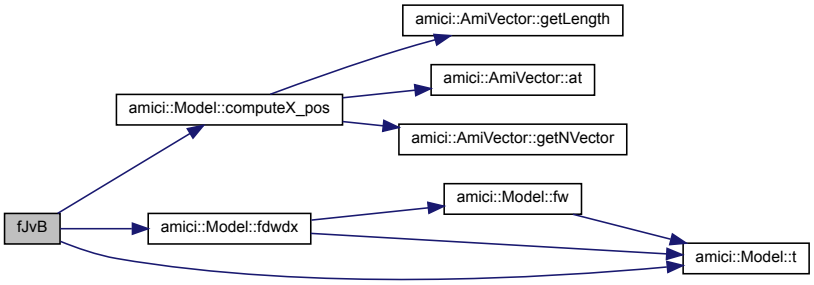
Matrix vector product of JB with a vector v (for iterative solvers)

Parameters

t	timepoint
x	Vector with the states
dx	Vector with the derivative states
xB	Vector with the adjoint states
dxB	Vector with the adjoint derivative states
vB	Vector with which the Jacobian is multiplied
JvB	Vector to which the Jacobian vector product will be written
cj	scalar in Jacobian (inverse stepsize)

Definition at line 204 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.11 froot() [1/3]

```
void froot (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            realtype * root )  [override], [virtual]
```

Root function

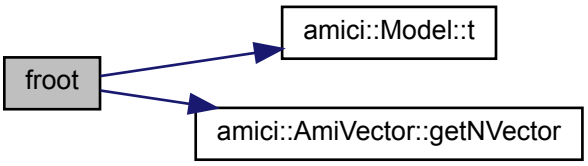
Parameters

t	time
x	state
dx	time derivative of state (DAE only)
root	array to which values of the root function will be written

Implements Model.

Definition at line 73 of file model_dae.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.12.3.12 froot() [2/3]

```
void froot (
            realtype t,
            N_Vector x,
            N_Vector dx,
            realtype * root )
```

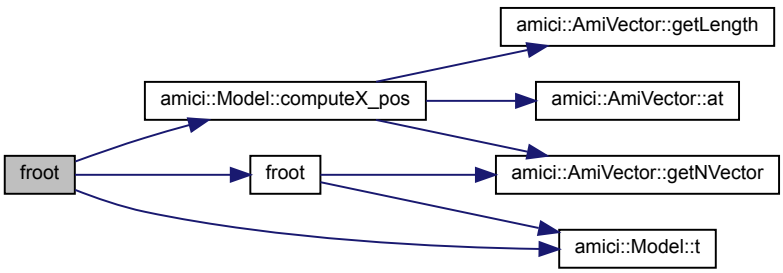
Event trigger function for events

Parameters

t	timepoint
x	Vector with the states
dx	Vector with the derivative states
root	array with root function values

Definition at line 83 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.13 fxdot() [1/3]

```
void fxdot (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot )  [override], [virtual]
```

Residual function

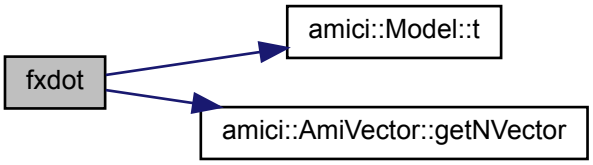
Parameters

t	time
x	state
dx	time derivative of state (DAE only)
xdot	array to which values of the residual function will be written

Implements Model.

Definition at line 90 of file model_dae.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.12.3.14 fxdot() [2/3]

```
void fxdot (
            realtype t,
            N_Vector x,
            N_Vector dx,
            N_Vector xdot )
```

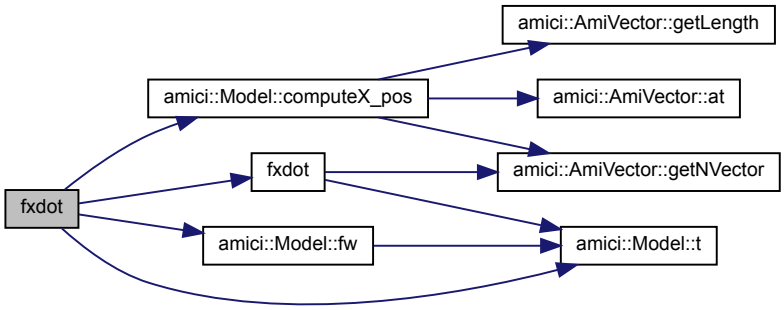
residual function of the DAE

Parameters

t	timepoint
x	Vector with the states
dx	Vector with the derivative states
xdot	Vector with the right hand side

Definition at line 100 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.15 fxBdot() [1/2]

```
void fxBdot (
            realtype t,
            N_Vector x,
            N_Vector dx,
            N_Vector xB,
            N_Vector dxB,
            N_Vector xBdot )
```

Right hand side of differential equation for adjoint state xB

Parameters

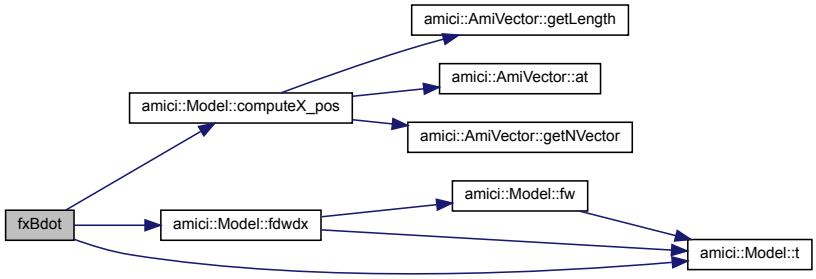
t	timepoint

Parameters

x	Vector with the states
dx	Vector with the derivative states
xB	Vector with the adjoint states
dxB	Vector with the adjoint derivative states
xBdot	Vector with the adjoint right hand side

Definition at line 222 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.16 fqBdot() [1/2]

```
void fqBdot (
            realtype t,
            N_Vector x,
            N_Vector dx,
            N_Vector xB,
            N_Vector dxB,
            N_Vector qBdot )
```

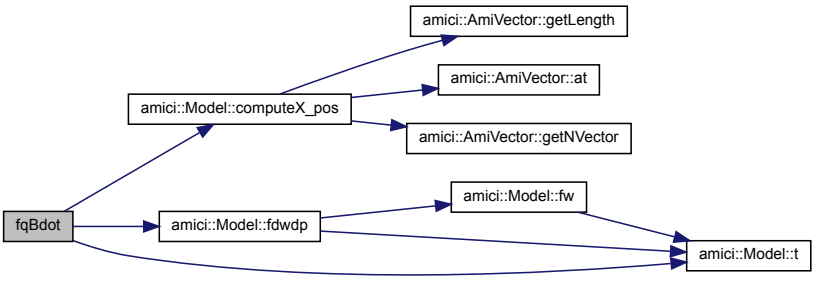
Right hand side of integral equation for quadrature states qB

Parameters

t	timepoint
x	Vector with the states
dx	Vector with the derivative states
xB	Vector with the adjoint states
dxB	Vector with the adjoint derivative states
qBdot	Vector with the adjoint quadrature right hand side

Definition at line 240 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.17 fdxdotdp() [1/3]

```
void fdxdotdp (
            const realtype t,
            const N_Vector x,
            const N_Vector dx )
```

Sensitivity of dx/dt wrt model parameters p

Parameters

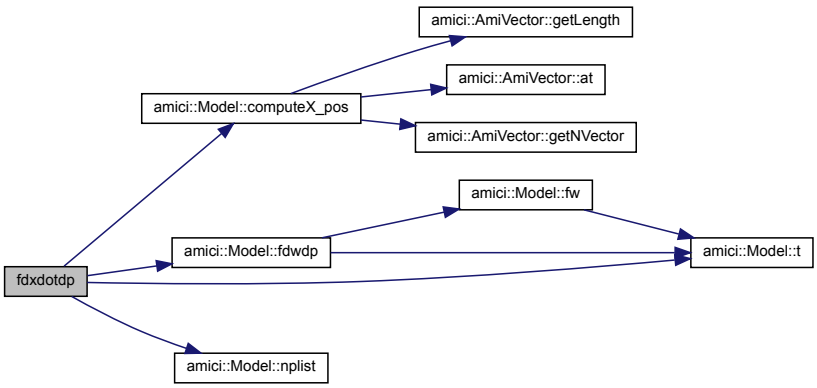
t	timepoint
x	Vector with the states
dx	Vector with the derivative states

Returns

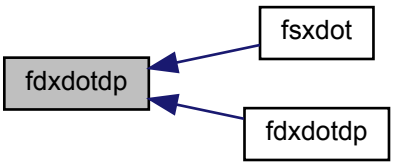
status flag indicating successful execution

Definition at line 133 of file model_dae.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.12.3.18 fdxdotdp() [2/3]

```
virtual void fdxdotdp (
            realtype t,
            AmiVector * x,
            AmiVector * dx )  [override], [virtual]
```

parameter derivative of residual function

Parameters

t	time
x	state
dx	time derivative of state (DAE only)

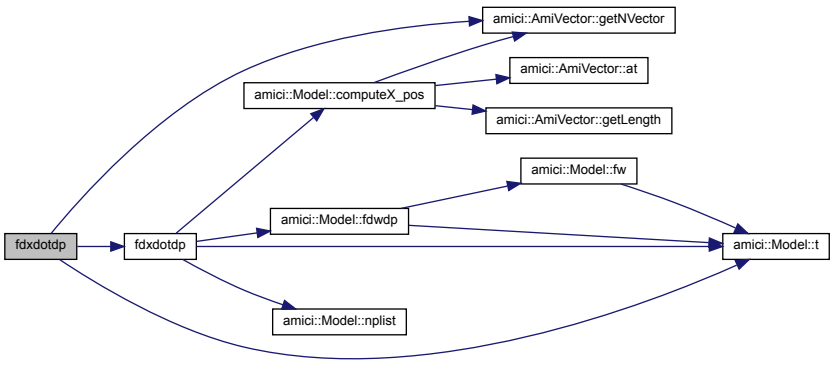
Returns

flag indicating successful evaluation

Implements Model.

Definition at line 98 of file model_dae.h.

Here is the call graph for this function:



10.12.3.19 fsxdot() [1/3]

```
void fsxdot (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            int ip,
            AmiVector * sx,
            AmiVector * sdx,
            AmiVector * sxdot )  [override], [virtual]
```

Sensitivity Residual function

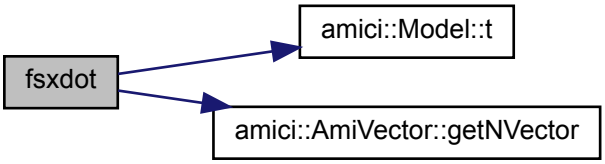
Parameters

t	time
x	state
dx	time derivative of state (DAE only)
ip	parameter index
sx	sensitivity state
sdx	time derivative of sensitivity state (DAE only)
sxdot	array to which values of the sensitivity residual function will be written

Implements Model.

Definition at line 250 of file model_dae.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.12.3.20 fsxdot() [2/3]

```
void fsxdot (
            realtype t,
            N_Vector x,
            N_Vector dx,
            int ip,
            N_Vector sx,
            N_Vector sdx,
            N_Vector sxdot )
```

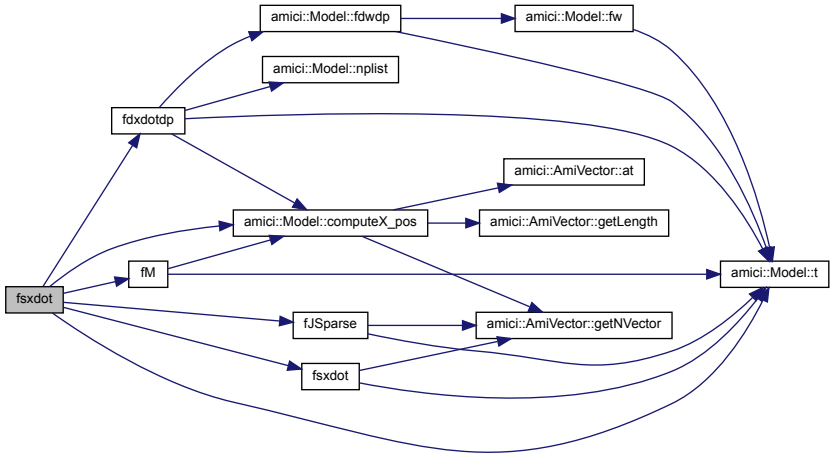
Right hand side of differential equation for state sensitivities sx

Parameters

t	timepoint
x	Vector with the states
dx	Vector with the derivative states
ip	parameter index
sx	Vector with the state sensitivities
sdx	Vector with the derivative state sensitivities
sxdot	Vector with the sensitivity right hand side

Definition at line 266 of file model_dae.cpp.

Here is the call graph for this function:



10.12.3.21 fM() [1/2]

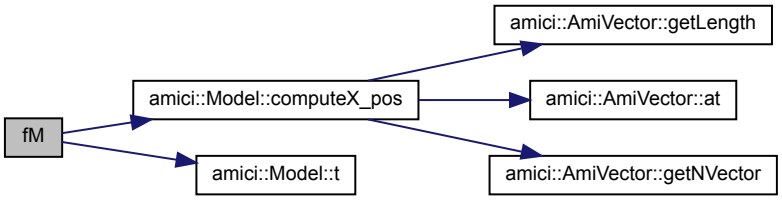
```
void fM (
            realtype t,
            const N_Vector x )
```

Parameters

t	timepoint
x	Vector with the states

Definition at line 147 of file model_dae.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.12.3.22 getSolver()

```
std::unique_ptr< Solver > getSolver ( ) [override], [virtual]
```

Retrieves the solver object

Returns

The Solver instance

Implements Model.

Definition at line 153 of file model_dae.cpp.

10.12.3.23 fJ() [3/3]

```
virtual void fJ (
            realtype * J,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype cj,
            const realtype * dx,
            const realtype * w,
            const realtype * dwdx ) [protected], [pure virtual]
```

model specific implementation for fJ

Parameters

J	Matrix to which the Jacobian will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
cj	scaling factor, inverse of the step size
dx	Vector with the derivative states
w	vector with helper variables
dwdx	derivative of w wrt x

10.12.3.24 fJB() [2/2]

```
virtual void fJB (
            realtype * JB,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype cj,
            const realtype * xB,
            const realtype * dx,
            const realtype * dxB,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJB

Parameters

JB	Matrix to which the Jacobian will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
cj	scaling factor, inverse of the step size
xB	Vector with the adjoint states
dx	Vector with the derivative states
dxB	Vector with the adjoint derivative states
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 142 of file model_dae.h.

10.12.3.25 fJSparse() [3/3]

```
virtual void fJSparse (
            SlsMat JSparse,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype cj,
            const realtype * dx,
            const realtype * w,
            const realtype * dwdx )  [protected], [pure virtual]
```

model specific implementation for fJSparse

Parameters

JSparse	Matrix to which the Jacobian will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
cj	scaling factor, inverse of the step size
dx	Vector with the derivative states
w	vector with helper variables
dwdx	derivative of w wrt x

10.12.3.26 fJSparseB() [2/2]

```
virtual void fJSparseB (
            SlsMat JSparseB,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype cj,
            const realtype * xB,
            const realtype * dx,
            const realtype * dxB,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJSparseB

Parameters

JSparseB	Matrix to which the Jacobian will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
cj	scaling factor, inverse of the step size
xB	Vector with the adjoint states
dx	Vector with the derivative states
dxB	Vector with the adjoint derivative states
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 177 of file model_dae.h.

10.12.3.27 fJDiag() [2/2]

```
virtual void fJDiag (
            realtype * JDiag,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype cj,
            const realtype * dx,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJDiag

Parameters

JDiag	array to which the Jacobian diagonal will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
cj	scaling factor, inverse of the step size
dx	Vector with the derivative states
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 195 of file model_dae.h.

10.12.3.28 fJv() [3/3]

```
virtual void fJv (
            realtype * Jv,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype cj,
            const realtype * dx,
            const realtype * v,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJv

Parameters

Jv	Matrix vector product of J with a vector v
t	timepoint

Parameters

x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
cj	scaling factor, inverse of the step size
dx	Vector with the derivative states
v	Vector with which the Jacobian is multiplied
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 213 of file model_dae.h.

10.12.3.29 fJvB() [2/2]

```
virtual void fJvB (
            realtype * JvB,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype cj,
            const realtype * xB,
            const realtype * dx,
            const realtype * dxB,
            const realtype * vB,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJvB

Parameters

JvB	Matrix vector product of JB with a vector v
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
cj	scaling factor, inverse of the step size
xB	Vector with the adjoint states
dx	Vector with the derivative states
dxB	Vector with the adjoint derivative states
vB	Vector with which the Jacobian is multiplied
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 234 of file model_dae.h.

10.12.3.30 froot() [3/3]

```
virtual void froot (
            realtype * root,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype * dx )  [protected], [virtual]
```

model specific implementation for froot

Parameters

root	values of the trigger function
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
dx	Vector with the derivative states

Definition at line 249 of file model_dae.h.

10.12.3.31 fxdot() [3/3]

```
virtual void fxdot (
            realtype * xdot,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype * dx,
            const realtype * w )  [protected], [pure virtual]
```

model specific implementation for fxdot

Parameters

xdot	residual function
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
w	vector with helper variables
dx	Vector with the derivative states

10.12.3.32 fxBdot() [2/2]

```
virtual void fxBdot (
            realtype * xBdot,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype * xB,
            const realtype * dx,
            const realtype * dxB,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fxBdot

Parameters

xBdot	adjoint residual function
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
xB	Vector with the adjoint states
dx	Vector with the derivative states
dxB	Vector with the adjoint derivative states
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 280 of file model_dae.h.

10.12.3.33 fqBdot() [2/2]

```
virtual void fqBdot (
            realtype * qBdot,
            const int ip,
            const realtype t,
            const realtype * x,
            const double * p,
            const double * k,
            const realtype * h,
            const realtype * xB,
            const realtype * dx,
            const realtype * dxB,
            const realtype * w,
            const realtype * dwdp )  [protected], [virtual]
```

model specific implementation for fqBdot

Parameters

qBdot	adjoint quadrature equation
ip	sensitivity index
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
xB	Vector with the adjoint states
dx	Vector with the derivative states
dxB	Vector with the adjoint derivative states
w	vector with helper variables
dwdp	derivative of w wrt p

Definition at line 300 of file model_dae.h.

10.12.3.34 fdxdotdp() [3/3]

```
virtual void fdxdotdp (
            realtype * dxdotdp,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ip,
            const realtype * dx,
            const realtype * w,
            const realtype * dwdp )  [protected], [virtual]
```

model specific implementation of fdxdotdp

Parameters

dxdotdp	partial derivative xdot wrt p
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
ip	parameter index
dx	Vector with the derivative states
w	vector with helper variables
dwdp	derivative of w wrt p

Definition at line 318 of file model_dae.h.

10.12.3.35 fsxdot() [3/3]

```
virtual void fsxdot (
            realtype * sxdot,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ip,
            const realtype * dx,
            const realtype * sx,
            const realtype * sdx,
            const realtype * w,
            const realtype * dwdx,
            const realtype * M,
            const realtype * J,
            const realtype * dxdotdp )  [protected], [virtual]
```

model specific implementation of fsxdot

Parameters

sxdot	sensitivity rhs
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
ip	parameter index
dx	Vector with the derivative states
sx	Vector with the state sensitivities
sdx	Vector with the derivative state sensitivities
w	vector with helper variables
dwdx	derivative of w wrt x
M	mass matrix
J	jacobian
dxdotdp	parameter derivative of residual function

Definition at line 340 of file model_dae.h.

10.12.3.36 fM() [2/2]

```
virtual void fM (
            realtype * M,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k )  [protected], [virtual]
```

model specific implementation of fM

Parameters

M	mass matrix
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector

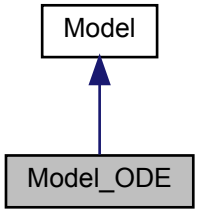
Definition at line 354 of file model_dae.h.

10.13 Model_ODE Class Reference

The Model class represents an AMICI ODE model. The model does not contain any data, but represents the state of the model at a specific time t. The states must not always be in sync, but may be updated asynchroneously.

```
#include <model_ode.h>
```

Inheritance diagram for Model_ODE:



Public Member Functions

- Model_ODE ()
- Model_ODE (const int nx_rdata, const int nxtrue_rdata, const int nx_solver, const int nxtrue_solver, const int ny, const int nytrue, const int nz, const int nztrue, const int ne, const int nJ, const int nw, const int ndwdx, const int ndwdp, const int nnz, const int ubw, const int lbw, const SecondOrderMode o2mode, const std::vector< realtype > p, const std::vector< realtype > k, const std::vector< int > plist, const std::vector< realtype > idlist, const std::vector< int > z2event)
- virtual void fJ (realtype t, realtype cj, AmiVector *x, AmiVector *dx, AmiVector *xdot, DlsMat J) override
- void fJ (realtype t, N_Vector x, N_Vector xdot, DlsMat J)
- void fJB (realtype t, N_Vector x, N_Vector xB, N_Vector xBdot, DlsMat JB)
- virtual void fJSparse (realtype t, realtype cj, AmiVector *x, AmiVector *dx, AmiVector *xdot, SlsMat J) override
- void fJSparse (realtype t, N_Vector x, SlsMat J)
- void fJSparseB (realtype t, N_Vector x, N_Vector xB, N_Vector xBdot, SlsMat JB)
- void fJDiag (realtype t, N_Vector JDiag, N_Vector x)
- virtual void fJDiag (realtype t, AmiVector *Jdiag, realtype cj, AmiVector *x, AmiVector *dx) override
- virtual void fJv (realtype t, AmiVector *x, AmiVector *dx, AmiVector *xdot, AmiVector *v, AmiVector *nJv, realtype cj) override
- void fJv (N_Vector v, N_Vector Jv, realtype t, N_Vector x)

- void fJvB (N_Vector vB, N_Vector JvB, realtype t, N_Vector x, N_Vector xB)
- virtual void froot (realtype t, AmiVector *x, AmiVector *dx, realtype *root) override
- void froot (realtype t, N_Vector x, realtype *root)
- virtual void fxdot (realtype t, AmiVector *x, AmiVector *dx, AmiVector *xdot) override
- void fxdot (realtype t, N_Vector x, N_Vector xdot)
- void fxBdot (realtype t, N_Vector x, N_Vector xB, N_Vector xBdot)
- void fqBdot (realtype t, N_Vector x, N_Vector xB, N_Vector qBdot)
- void fdxdotdp (const realtype t, const N_Vector x)
- virtual void fdxdotdp (realtype t, AmiVector *x, AmiVector *dx) override
- void fsxdot (realtype t, AmiVector *x, AmiVector *dx, int ip, AmiVector *sx, AmiVector *sdx, AmiVector *sxdot) override
- void fsxdot (realtype t, N_Vector x, int ip, N_Vector sx, N_Vector sxdot)
- virtual std::unique_ptr< Solver > getSolver () override

Protected Member Functions

- virtual void fJ (realtype *J, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *w, const realtype *dwdx)=0
- virtual void fJB (realtype *JB, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *xB, const realtype *w, const realtype *dwdx)
- virtual void fJSparse (SlsMat JSparse, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *w, const realtype *dwdx)=0
- virtual void fJSparseB (SlsMat JSparseB, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *xB, const realtype *w, const realtype *dwdx)
- virtual void fJDiag (realtype *JDiag, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *w, const realtype *dwdx)
- virtual void fJv (realtype *Jv, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *v, const realtype *w, const realtype *dwdx)
- virtual void fJvB (realtype *JvB, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *xB, const realtype *vB, const realtype *w, const realtype *dwdx)
- virtual void froot (realtype *root, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h)
- virtual void fxdot (realtype *xdot, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *w)=0
- virtual void fxBdot (realtype *xBdot, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *xB, const realtype *w, const realtype *dwdx)
- virtual void fqBdot (realtype *qBdot, const int ip, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const realtype *xB, const realtype *w, const realtype *dwdp)
- virtual void fdxdotdp (realtype *dxdotdp, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const int ip, const realtype *w, const realtype *dwdp)
- virtual void fsxdot (realtype *sxdot, const realtype t, const realtype *x, const realtype *p, const realtype *k, const realtype *h, const int ip, const realtype *sx, const realtype *w, const realtype *dwdx, const realtype *J, const realtype *dxdotdp)

Additional Inherited Members

10.13.1 Detailed Description

Definition at line 23 of file model_ode.h.

10.13.2 Constructor & Destructor Documentation

10.13.2.1 Model_ODE() [1/2]

```
Model_ODE ( )
```

default constructor

Definition at line 26 of file model_ode.h.

10.13.2.2 Model_ODE() [2/2]

```
Model_ODE (
            const int nx_rdata,
            const int nxtrue_rdata,
            const int nx_solver,
            const int nxtrue_solver,
            const int ny,
            const int nytrue,
            const int nz,
            const int nztrue,
            const int ne,
            const int nJ,
            const int nw,
            const int ndwdx,
            const int ndwdp,
            const int nnz,
            const int ubw,
            const int lbw,
            const SecondOrderMode o2mode,
            const std::vector< realtype > p,
            const std::vector< realtype > k,
            const std::vector< int > plist,
            const std::vector< realtype > idlist,
            const std::vector< int > z2event )
```

constructor with model dimensions

Parameters

nx_rdata	number of state variables
nxtrue_rdata	number of state variables of the non-augmented model
nx_solver	number of state variables with conservation laws applied
nxtrue_solver	number of state variables of the non-augmented model with conservation laws applied
ny	number of observables
nytrue	number of observables of the non-augmented model
nz	number of event observables
nztrue	number of event observables of the non-augmented model
ne	number of events
nJ	number of objective functions
nw	number of repeating elements
ndwdx	number of nonzero elements in the x derivative of the repeating elements
ndwdp	number of nonzero elements in the p derivative of the repeating elements
nnz	number of nonzero elements in Jacobian
ubw	upper matrix bandwidth in the Jacobian

Parameters

lbw	lower matrix bandwidth in the Jacobian
o2mode	second order sensitivity mode
p	parameters
k	constants
plist	indexes wrt to which sensitivities are to be computed
idlist	indexes indicating algebraic components (DAE only)
z2event	mapping of event outputs to events

Definition at line 55 of file model_ode.h.

10.13.3 Member Function Documentation

10.13.3.1 fJ() [1/3]

```
void fJ (
            realtype t,
            realtype cj,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot,
            DlsMat J )  [override], [virtual]
```

Dense Jacobian function

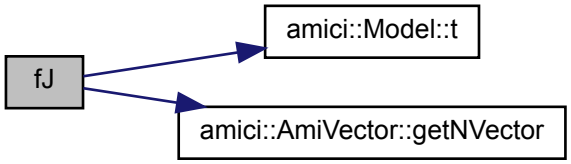
Parameters

t	time
cj	scaling factor (inverse of timestep, DAE only)
x	state
dx	time derivative of state (DAE only)
xdot	values of residual function (unused)
J	dense matrix to which values of the jacobian will be written

Implements Model.

Definition at line 6 of file model_ode.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.13.3.2 fJ() [2/3]

```
void fJ (
            realtype t,
            N_Vector x,
            N_Vector xdot,
            DlsMat J )
```

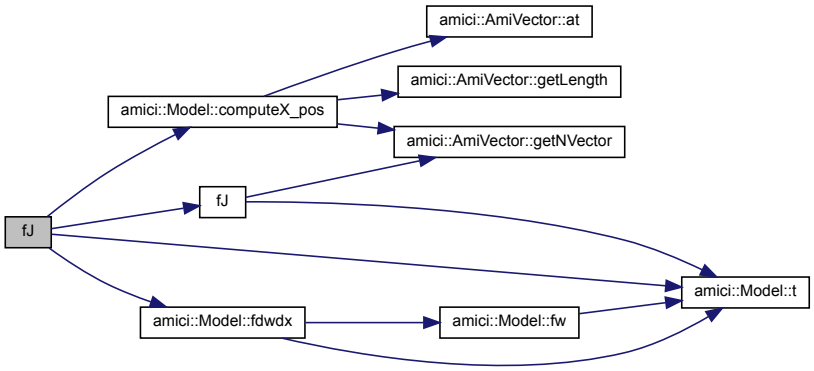
implementation of fJ at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation aswell as the AmiVector level implementation

Parameters

t	timepoint
x	Vector with the states
xdot	Vector with the right hand side
J	Matrix to which the Jacobian will be written

Definition at line 20 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.3 fJB() [1/2]

```
void fJB (
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector xBdot,
            DlsMat JB )
```

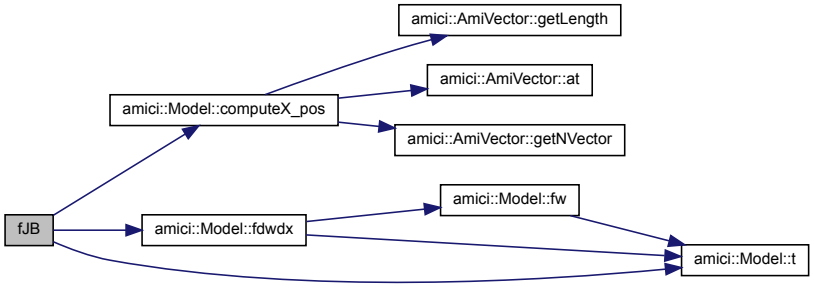
implementation of fJB at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation

Parameters

t	timepoint
x	Vector with the states
xB	Vector with the adjoint states
xBdot	Vector with the adjoint right hand side
JB	Matrix to which the Jacobian will be written

Definition at line 147 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.4 fJSparse() [1/3]

```
void fJSparse (
            realtype t,
            realtype cj,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot,
            SlsMat J )  [override], [virtual]
```

Sparse Jacobian function

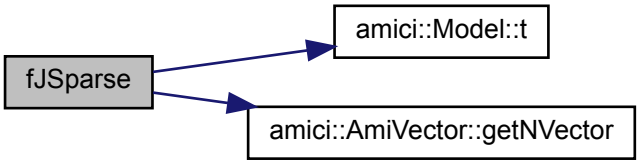
Parameters

t	time
cj	scaling factor (inverse of timestep, DAE only)
x	state
dx	time derivative of state (DAE only)
xdot	values of residual function (unused)
J	sparse matrix to which values of the Jacobian will be written

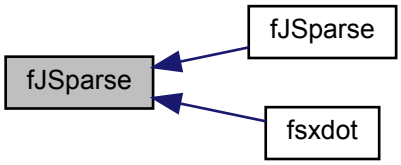
Implements Model.

Definition at line 28 of file model_ode.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.13.3.5 fJSparse() [2/3]

```
void fJSparse (
            realtype t,
            N_Vector x,
            SlsMat J )
```

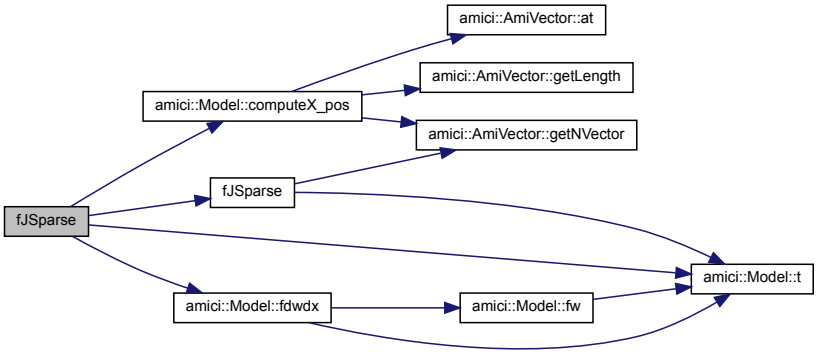
implementation of fJSparse at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation aswell as the AmiVector level implementation

Parameters

t	timepoint
x	Vector with the states
J	Matrix to which the Jacobian will be written

Definition at line 40 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.6 fJSparseB() [1/2]

```
void fJSparseB (
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector xBdot,
            SlsMat JB )
```

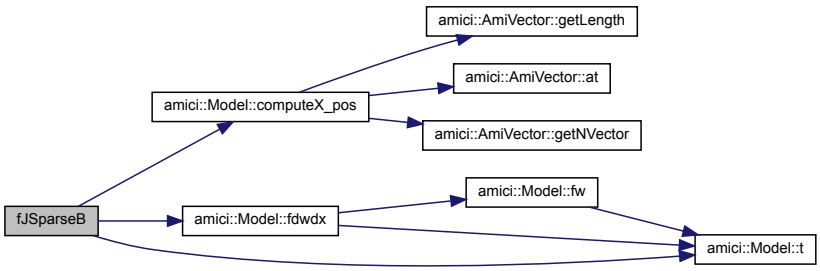
implementation of fJSparseB at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation

Parameters

t	timepoint
x	Vector with the states
xB	Vector with the adjoint states
xBdot	Vector with the adjoint right hand side
JB	Matrix to which the Jacobian will be written

Definition at line 164 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.7 fJDiag() [1/3]

```
void fJDiag (
            realtype t,
            N_Vector JDiag,
            N_Vector x )
```

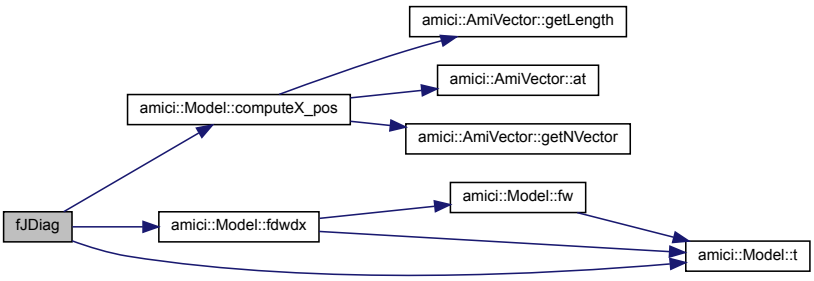
implementation of fJDiag at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation

Parameters

t	timepoint
JDiag	Vector to which the Jacobian diagonal will be written
x	Vector with the states

Definition at line 178 of file model_ode.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.13.3.8 fJDiag() [2/3]

```
void fJDiag (
            realtype t,
            AmiVector * JDiag,
            realtype cj,
            AmiVector * x,
            AmiVector * dx )  [override], [virtual]
```

diagonalized Jacobian (for preconditioning)

Parameters

t	timepoint
JDiag	Vector to which the Jacobian diagonal will be written
cj	scaling factor, inverse of the step size
x	Vector with the states
dx	Vector with the derivative states

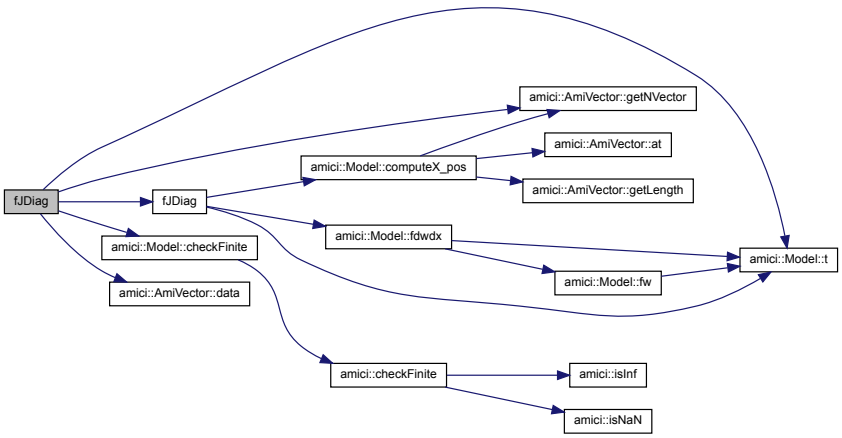
Returns

status flag indicating successful execution

Implements Model.

Definition at line 114 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.9 fJv() [1/3]

```
void fJv (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot,
            AmiVector * v,
            AmiVector * nJv,
            realtype cj )  [override], [virtual]
```

Jacobian multiply function

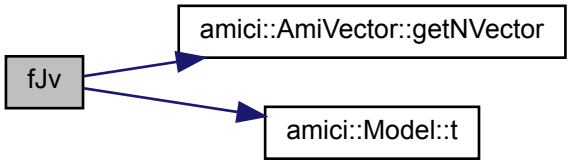
Parameters

t	time
x	state
dx	time derivative of state (DAE only)
xdot	values of residual function (unused)
v	multiplication vector (unused)
nJv	array to which result of multiplication will be written
cj	scaling factor (inverse of timestep, DAE only)

Implements Model.

Definition at line 48 of file model_ode.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.13.3.10 fJv() [2/3]

```
void fJv (
            N_Vector v,
            N_Vector Jv,
            realtype t,
            N_Vector x )
```

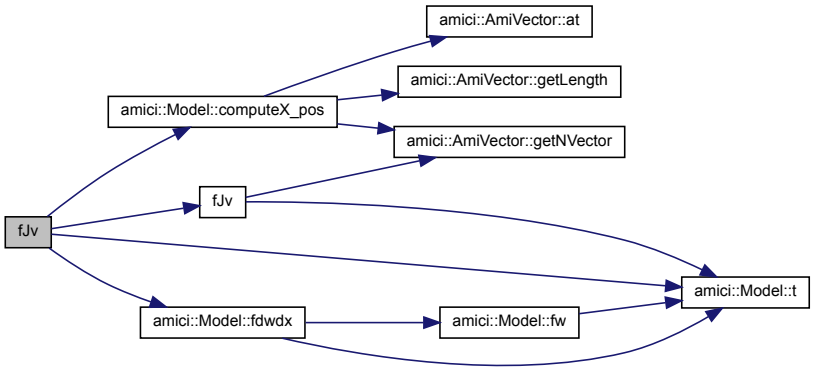
implementation of fJv at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation aswell as the AmiVector level implementation

Parameters

t	timepoint
x	Vector with the states
v	Vector with which the Jacobian is multiplied
Jv	Vector to which the Jacobian vector product will be written

Definition at line 62 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.11 fJvB() [1/2]

```
void fJvB (
            N_Vector vB,
            N_Vector JvB,
            realtype t,
            N_Vector x,
            N_Vector xB )
```

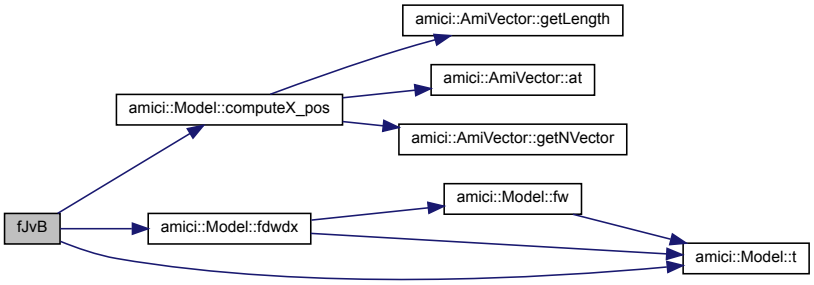
implementation of fJvB at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation

Parameters

t	timepoint
x	Vector with the states
xB	Vector with the adjoint states
vB	Vector with which the Jacobian is multiplied
JvB	Vector to which the Jacobian vector product will be written

Definition at line 195 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.12 froot() [1/3]

```
void froot (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            realtype * root )  [override], [virtual]
```

Root function

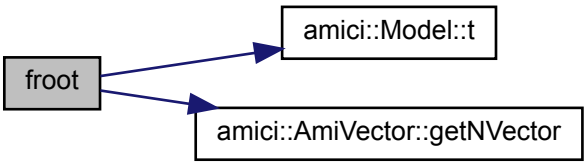
Parameters

t	time
x	state
dx	time derivative of state (DAE only)
root	array to which values of the root function will be written

Implements Model.

Definition at line 70 of file model_ode.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.13.3.13 froot() [2/3]

```
void froot (
            realtype t,
            N_Vector x,
            realtype * root )
```

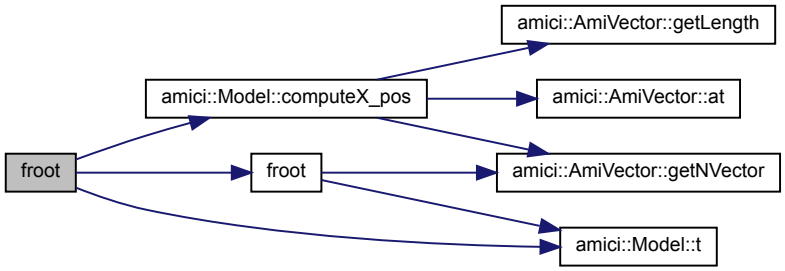
implementation of froot at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation aswell as the AmiVector level implementation

Parameters

t	timepoint
x	Vector with the states
root	array with root function values

Definition at line 81 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.14 fxdot() [1/3]

```
void fxdot (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            AmiVector * xdot )  [override], [virtual]
```

Residual function

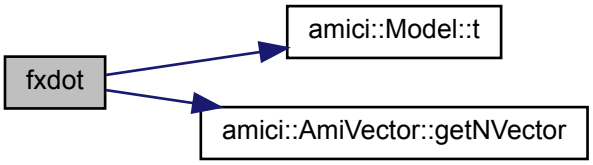
Parameters

t	time
x	state
dx	time derivative of state (DAE only)
xdot	array to which values of the residual function will be written

Implements Model.

Definition at line 87 of file model_ode.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.13.3.15 fxdot() [2/3]

```
void fxdot (
            realtype t,
            N_Vector x,
            N_Vector xdot )
```

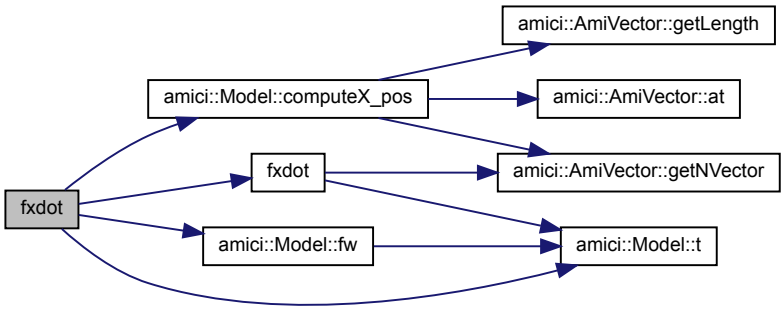
implementation of fxdot at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation aswell as the AmiVector level implementation

Parameters

t	timepoint
x	Vector with the states
xdot	Vector with the right hand side

Definition at line 98 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.16 fxBdot() [1/2]

```
void fxBdot (
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector xBdot )
```

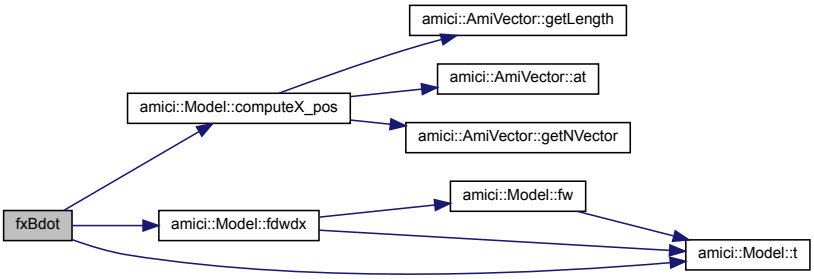
implementation of fxBdot at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation

Parameters

t	timepoint
x	Vector with the states
xB	Vector with the adjoint states
xBdot	Vector with the adjoint right hand side

Definition at line 210 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.17 fqBdot() [1/2]

```
void fqBdot (
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector qBdot )
```

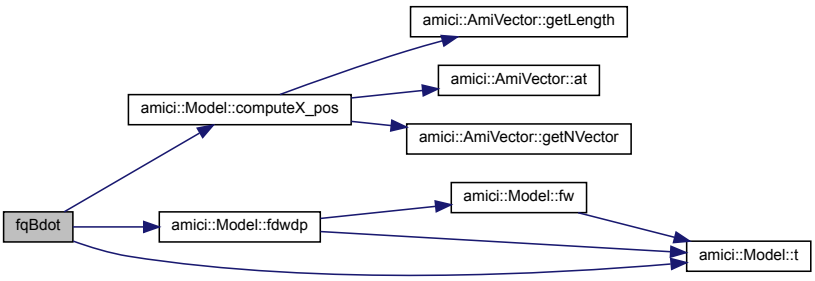
implementation of fqBdot at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation

Parameters

t	timepoint
x	Vector with the states
xB	Vector with the adjoint states
qBdot	Vector with the adjoint quadrature right hand side

Definition at line 225 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.18 fdxdotdp() [1/3]

```
void fdxdotdp (
            const realtype t,
            const N_Vector x )
```

Sensitivity of dx/dt wrt model parameters p

Parameters

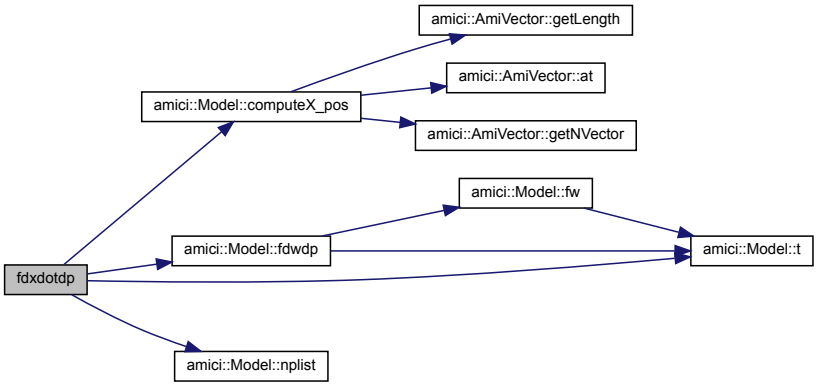
t	timepoint
x	Vector with the states

Returns

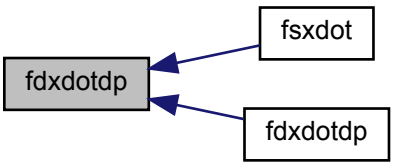
status flag indicating successful execution

Definition at line 126 of file model_ode.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.13.3.19 fdxdotdp() [2/3]

```
virtual void fdxdotdp (
            realtype t,
            AmiVector * x,
            AmiVector * dx )  [override], [virtual]
```

parameter derivative of residual function

Parameters

t	time
x	state
dx	time derivative of state (DAE only)

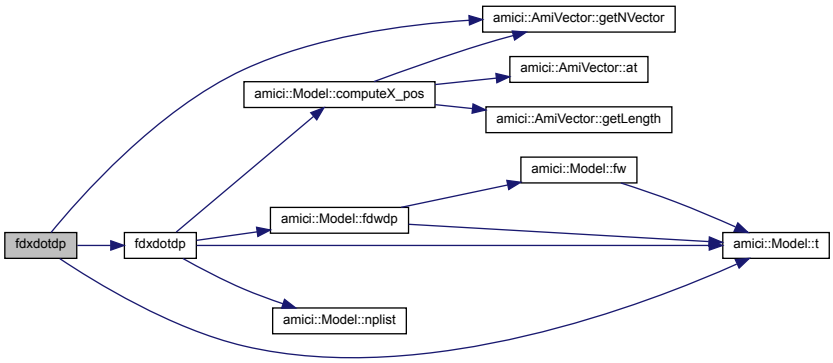
Returns

flag indicating successful evaluation

Implements Model.

Definition at line 99 of file model_ode.h.

Here is the call graph for this function:



10.13.3.20 fsxdot() [1/3]

```
void fsxdot (
            realtype t,
            AmiVector * x,
            AmiVector * dx,
            int ip,
            AmiVector * sx,
            AmiVector * sdx,
            AmiVector * sxdot )  [override], [virtual]
```

Sensitivity Residual function

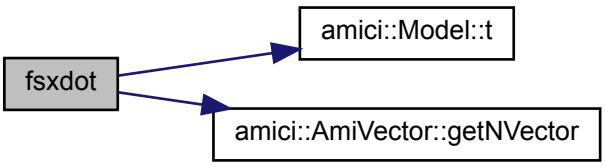
Parameters

t	time
x	state
dx	time derivative of state (DAE only)
ip	parameter index
sx	sensitivity state
sdx	time derivative of sensitivity state (DAE only)
sxdot	array to which values of the sensitivity residual function will be written

Implements Model.

Definition at line 235 of file model_ode.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.13.3.21 fsxdot() [2/3]

```
void fsxdot (
            realtype t,
            N_Vector x,
            int ip,
            N_Vector sx,
            N_Vector sxdot )
```

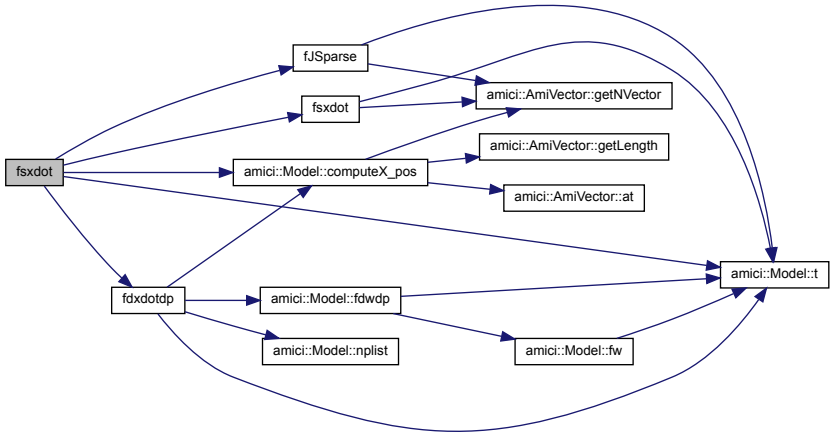
implementation of fsxdot at the N_Vector level, this function provides an interface to the model specific routines for the solver implementation

Parameters

t	timepoint
x	Vector with the states
ip	parameter index
sx	Vector with the state sensitivities
sxdot	Vector with the sensitivity right hand side

Definition at line 248 of file model_ode.cpp.

Here is the call graph for this function:



10.13.3.22 getSolver()

```
std::unique_ptr< Solver > getSolver ( ) [override], [virtual]
```

Retrieves the solver object

Returns

The Solver instance

Implements Model.

Definition at line 135 of file model_ode.cpp.

10.13.3.23 fJ() [3/3]

```
virtual void fJ (
            realtype * J,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * w,
            const realtype * dwdx ) [protected], [pure virtual]
```

model specific implementation for fJ

Parameters

J	Matrix to which the Jacobian will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
w	vector with helper variables
dwdx	derivative of w wrt x

10.13.3.24 fJB() [2/2]

```
virtual void fJB (
            realtype * JB,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * xB,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJB

Parameters

JB	Matrix to which the Jacobian will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
xB	Vector with the adjoint states
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 134 of file model_ode.h.

10.13.3.25 fJSparse() [3/3]

```
virtual void fJSparse (
            SlsMat JSparse,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
```

```
            const realtype * h,
            const realtype * w,
            const realtype * dwdx )  [protected], [pure virtual]
```

model specific implementation for fJSparse

Parameters

JSparse	Matrix to which the Jacobian will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
w	vector with helper variables
dwdx	derivative of w wrt x

10.13.3.26 fJSparseB() [2/2]

```
virtual void fJSparseB (
            SlsMat JSparseB,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * xB,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJSparseB

Parameters

JSparseB	Matrix to which the Jacobian will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
xB	Vector with the adjoint states
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 162 of file model_ode.h.

10.13.3.27 fJDiag() [3/3]

```
virtual void fJDiag (
            realtype * JDiag,
```

```
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJDiag

Parameters

JDiag	Matrix to which the Jacobian will be written
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 177 of file model_ode.h.

10.13.3.28 fJv() [3/3]

```
virtual void fJv (
            realtype * Jv,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * v,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJv

Parameters

Jv	Matrix vector product of J with a vector v
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
v	Vector with which the Jacobian is multiplied
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 193 of file model_ode.h.

10.13.3.29 fJvB() [2/2]

```
virtual void fJvB (
            realtype * JvB,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * xB,
            const realtype * vB,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fJvB

Parameters

JvB	Matrix vector product of JB with a vector v
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
xB	Vector with the adjoint states
vB	Vector with which the Jacobian is multiplied
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 210 of file model_ode.h.

10.13.3.30 froot() [3/3]

```
virtual void froot (
            realtype * root,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h )  [protected], [virtual]
```

model specific implementation for froot

Parameters

root	values of the trigger function
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector

Definition at line 223 of file model_ode.h.

10.13.3.31 fxdot() [3/3]

```
virtual void fxdot (
            realtype * xdot,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * w )  [protected], [pure virtual]
```

model specific implementation for fxdot

Parameters

xdot	residual function
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
w	vector with helper variables

10.13.3.32 fxBdot() [2/2]

```
virtual void fxBdot (
            realtype * xBdot,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * xB,
            const realtype * w,
            const realtype * dwdx )  [protected], [virtual]
```

model specific implementation for fxBdot

Parameters

xBdot	adjoint residual function
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
xB	Vector with the adjoint states
w	vector with helper variables
dwdx	derivative of w wrt x

Definition at line 249 of file model_ode.h.

10.13.3.33 fqBdot() [2/2]

```
virtual void fqBdot (
            realtype * qBdot,
            const int ip,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const realtype * xB,
            const realtype * w,
            const realtype * dwdp )  [protected], [virtual]
```

model specific implementation for fqBdot

Parameters

qBdot	adjoint quadrature equation
ip	sensitivity index
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
xB	Vector with the adjoint states
w	vector with helper variables
dwdp	derivative of w wrt p

Definition at line 266 of file model_ode.h.

10.13.3.34 fdxdotdp() [3/3]

```
virtual void fdxdotdp (
            realtype * dxdotdp,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ip,
            const realtype * w,
            const realtype * dwdp )  [protected], [virtual]
```

model specific implementation of fdxdotdp

Parameters

dxdotdp	partial derivative xdot wrt p
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
ip	parameter index
w	vector with helper variables
dwdp	derivative of w wrt p

Definition at line 282 of file model_ode.h.

10.13.3.35 fsxdot() [3/3]

```
virtual void fsxdot (
            realtype * sxdot,
            const realtype t,
            const realtype * x,
            const realtype * p,
            const realtype * k,
            const realtype * h,
            const int ip,
            const realtype * sx,
            const realtype * w,
            const realtype * dwdx,
            const realtype * J,
            const realtype * dxdotdp )  [protected], [virtual]
```

model specific implementation of fsxdot

Parameters

sxdot	sensitivity rhs
t	timepoint
x	Vector with the states
p	parameter vector
k	constants vector
h	heavyside vector
ip	parameter index
sx	Vector with the state sensitivities
w	vector with helper variables
dwdx	derivative of w wrt x
J	jacobian
dxdotdp	parameter derivative of residual function

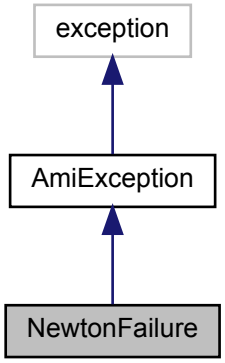
Definition at line 301 of file model_ode.h.

10.14 NewtonFailure Class Reference

newton failure exception this exception should be thrown when the steady state computation failed to converge for this exception we can assume that we can recover from the exception and return a solution struct to the user

```
#include <exception.h>
```

Inheritance diagram for NewtonFailure:



Public Member Functions

- NewtonFailure (int code, const char *function)

Public Attributes

- int error_code

10.14.1 Detailed Description

Definition at line 201 of file exception.h.

10.14.2 Constructor & Destructor Documentation

10.14.2.1 NewtonFailure()

```
NewtonFailure (
            int code,
            const char * function )
```

constructor, simply calls AmiException constructor

Parameters

function	name of the function in which the error occured
code	error code

Definition at line 209 of file exception.h.

10.14.3 Member Data Documentation

10.14.3.1 error_code

```
int error_code
```

error code returned by solver

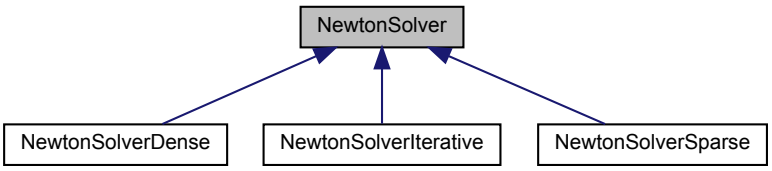
Definition at line 204 of file exception.h.

10.15 NewtonSolver Class Reference

The NewtonSolver class sets up the linear solver for the Newton method.

```
#include <newton_solver.h>
```

Inheritance diagram for NewtonSolver:



Public Member Functions

- NewtonSolver (realtype ∗t, AmiVector ∗x, Model ∗model, ReturnData ∗rdata)
- void getStep (int ntry, int nnewt, AmiVector ∗delta)
- void computeNewtonSensis (AmiVectorArray ∗sx)
- virtual void prepareLinearSystem (int ntry, int nnewt)=0
- virtual void solveLinearSystem (AmiVector ∗rhs)=0

Static Public Member Functions

- static std::unique_ptr< NewtonSolver > getSolver (realtype ∗t, AmiVector ∗x, LinearSolver linsolType, Model ∗model, ReturnData ∗rdata, int maxlinsteps, int maxsteps, double atol, double rtol)

Public Attributes

- int maxlinsteps = 0
- int maxsteps = 0
- double atol = 1e-16
- double rtol = 1e-8

Protected Attributes

- realtype * t
- Model * model
- ReturnData * rdata
- AmiVector xdot
- AmiVector * x
- AmiVector dx

10.15.1 Detailed Description

Definition at line 25 of file newton_solver.h.

10.15.2 Constructor & Destructor Documentation

10.15.2.1 NewtonSolver()

```
NewtonSolver (
            realtype * t,
            AmiVector * x,
            Model * model,
            ReturnData * rdata )
```

default constructor, initializes all members with the provided objects

Parameters

t	pointer to time variable
x	pointer to state variables
model	pointer to the AMICI model object
rdata	pointer to the return data object

Definition at line 18 of file newton_solver.cpp.

10.15.3 Member Function Documentation

10.15.3.1 getSolver()

```
std::unique_ptr< NewtonSolver > getSolver (
            realtype * t,
            AmiVector * x,
            LinearSolver linsolType,
            Model * model,
            ReturnData * rdata,
            int maxlinsteps,
            int maxsteps,
            double atol,
            double rtol )  [static]
```

Tries to determine the steady state of the ODE system by a Newton solver, uses forward intergration, if the Newton solver fails, restarts Newton solver, if integration fails. Computes steady state sensitivities

Parameters

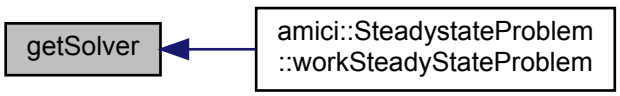
t	pointer to time variable
x	pointer to state variables
linsolType	integer indicating which linear solver to use
model	pointer to the AMICI model object
rdata	pointer to the return data object
maxlinsteps	maximum number of allowed linear steps per Newton step for steady state computation
maxsteps	maximum number of allowed Newton steps for steady state computation
atol	absolute tolerance
rtol	relative tolerance

Returns

solver NewtonSolver according to the specified linsolType

Definition at line 36 of file newton_solver.cpp.

Here is the caller graph for this function:



10.15.3.2 getStep()

```
void getStep (
            int ntry,
            int nnewt,
            AmiVector * delta )
```

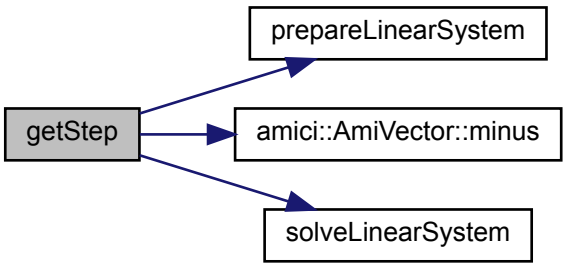
Computes the solution of one Newton iteration

Parameters

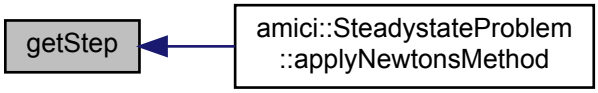
ntry	integer newton_try integer start number of Newton solver (1 or 2)
nnewt	integer number of current Newton step
delta	containing the RHS of the linear system, will be overwritten by solution to the linear system

Definition at line 107 of file newton_solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.15.3.3 computeNewtonSensis()

```
void computeNewtonSensis (
            AmiVectorArray * sx )
```

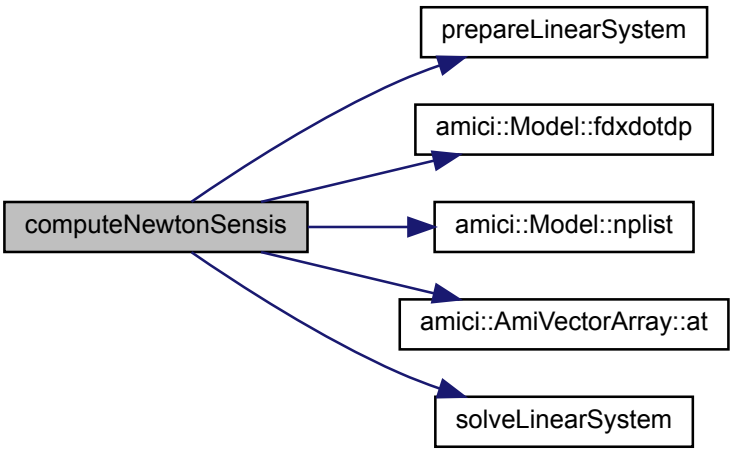
Computes steady state sensitivities

Parameters

sx	pointer to state variable sensitivities

Definition at line 127 of file newton_solver.cpp.

Here is the call graph for this function:



10.15.3.4 prepareLinearSystem()

```
virtual void prepareLinearSystem (
            int ntry,
            int nnewt )  [pure virtual]
```

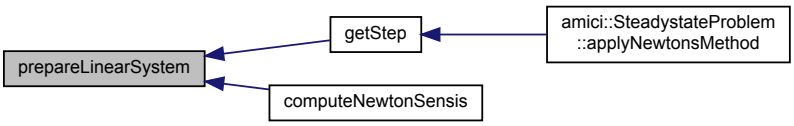
Writes the Jacobian for the Newton iteration and passes it to the linear solver

Parameters

ntry	integer newton_try integer start number of Newton solver (1 or 2)
nnewt	integer number of current Newton step

Implemented in NewtonSolverIterative, NewtonSolverSparse, and NewtonSolverDense.

Here is the caller graph for this function:



10.15.3.5 solveLinearSystem()

```
virtual void solveLinearSystem (
            AmiVector * rhs )  [pure virtual]
```

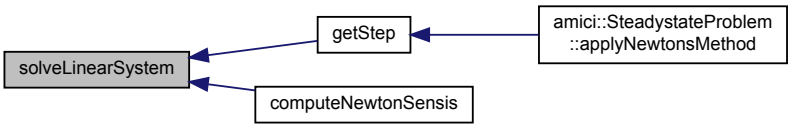
Solves the linear system for the Newton step

Parameters

rhs	containing the RHS of the linear system, will be overwritten by solution to the linear system

Implemented in NewtonSolverIterative, NewtonSolverSparse, and NewtonSolverDense.

Here is the caller graph for this function:



10.15.4 Member Data Documentation

10.15.4.1 maxlinsteps

```
int maxlinsteps = 0
```

maximum number of allowed linear steps per Newton step for steady state computation

Definition at line 59 of file newton_solver.h.

10.15.4.2 maxsteps

```
int maxsteps = 0
```

maximum number of allowed Newton steps for steady state computation

Definition at line 61 of file newton_solver.h.

10.15.4.3 atol

```
double atol = 1e-16
```

absolute tolerance

Definition at line 63 of file newton_solver.h.

10.15.4.4 rtol

```
double rtol = 1e-8
```

relative tolerance

Definition at line 65 of file newton_solver.h.

10.15.4.5 t

```
realtype* t  [protected]
```

time variable

Definition at line 69 of file newton_solver.h.

10.15.4.6 model

```
Model* model  [protected]
```

pointer to the AMICI model object

Definition at line 71 of file newton_solver.h.

10.15.4.7 rdata

```
ReturnData* rdata  [protected]
```

pointer to the return data object

Definition at line 73 of file newton_solver.h.

10.15.4.8 xdot

```
AmiVector xdot [protected]
```

right hand side AmiVector

Definition at line 75 of file newton_solver.h.

10.15.4.9 x

```
AmiVector* x [protected]
```

current state

Definition at line 77 of file newton_solver.h.

10.15.4.10 dx

```
AmiVector dx [protected]
```

current state time derivative (DAE)

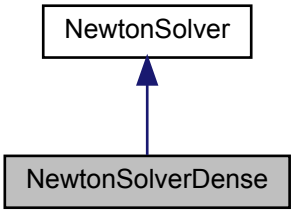
Definition at line 79 of file newton_solver.h.

10.16 NewtonSolverDense Class Reference

The NewtonSolverDense provides access to the dense linear solver for the Newton method.

```
#include <newton_solver.h>
```

Inheritance diagram for NewtonSolverDense:



Public Member Functions

- NewtonSolverDense (realtype *t, AmiVector *x, Model *model, ReturnData *rdata)
- void solveLinearSystem (AmiVector *rhs) override
- void prepareLinearSystem (int ntry, int nnewt) override

Additional Inherited Members

10.16.1 Detailed Description

Definition at line 88 of file newton_solver.h.

10.16.2 Constructor & Destructor Documentation

10.16.2.1 NewtonSolverDense()

```
NewtonSolverDense (
            realtype * t,
            AmiVector * x,
            Model * model,
            ReturnData * rdata )
```

default constructor, initializes all members with the provided objects and initializes temporary storage objects

Parameters

t	pointer to time variable
x	pointer to state variables
model	pointer to the AMICI model object
rdata	pointer to the return data object

Definition at line 152 of file newton_solver.cpp.

10.16.3 Member Function Documentation

10.16.3.1 solveLinearSystem()

```
void solveLinearSystem (
            AmiVector * rhs )  [override], [virtual]
```

Solves the linear system for the Newton step

Parameters

rhs	containing the RHS of the linear system, will be overwritten by solution to the linear system

Solves the linear system for the Newton step

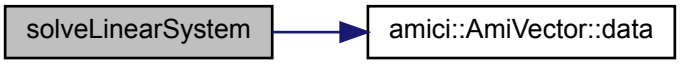
Parameters

rhs	containing the RHS of the linear system, will be overwritten by solution to the linear system

Implements NewtonSolver.

Definition at line 191 of file newton_solver.cpp.

Here is the call graph for this function:



10.16.3.2 prepareLinearSystem()

```
void prepareLinearSystem (
            int ntry,
            int nnewt )  [override], [virtual]
```

Writes the Jacobian for the Newton iteration and passes it to the linear solver

Parameters

ntry	integer newton_try integer start number of Newton solver (1 or 2)
nnewt	integer number of current Newton step

Writes the Jacobian for the Newton iteration and passes it to the linear solver

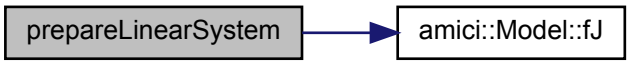
Parameters

ntry	integer newton_try integer start number of Newton solver (1 or 2)
nnewt	integer number of current Newton step

Implements NewtonSolver.

Definition at line 171 of file newton_solver.cpp.

Here is the call graph for this function:

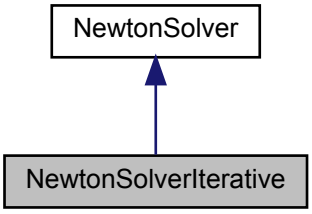


10.17 NewtonSolverIterative Class Reference

The NewtonSolverIterative provides access to the iterative linear solver for the Newton method.

```
#include <newton_solver.h>
```

Inheritance diagram for NewtonSolverIterative:



Public Member Functions

- NewtonSolverIterative (realtype *t, AmiVector *x, Model *model, ReturnData *rdata)
- void solveLinearSystem (AmiVector *rhs)
- void prepareLinearSystem (int ntry, int nnewt)
- void linsolveSPBCG (int ntry, int nnewt, AmiVector *ns_delta)

Additional Inherited Members

10.17.1 Detailed Description

Definition at line 136 of file newton_solver.h.

10.17.2 Constructor & Destructor Documentation

10.17.2.1 NewtonSolverIterative()

```
NewtonSolverIterative (
            realtype * t,
            AmiVector * x,
            Model * model,
            ReturnData * rdata )
```

default constructor, initializes all members with the provided objects

Parameters

t	pointer to time variable
x	pointer to state variables
model	pointer to the AMICI model object
rdata	pointer to the return data object

Definition at line 312 of file newton_solver.cpp.

10.17.3 Member Function Documentation

10.17.3.1 solveLinearSystem()

```
void solveLinearSystem (
            AmiVector * rhs )  [virtual]
```

Solves the linear system for the Newton step

Parameters

rhs	containing the RHS of the linear system, will be overwritten by solution to the linear system

Solves the linear system for the Newton step by passing it to linsolveSPBCG

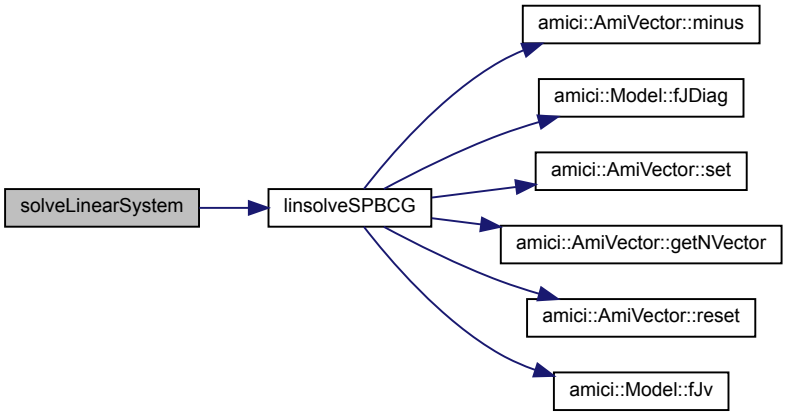
Parameters

rhs	containing the RHS of the linear system, will be overwritten by solution to the linear system

Implements NewtonSolver.

Definition at line 350 of file newton_solver.cpp.

Here is the call graph for this function:



10.17.3.2 prepareLinearSystem()

```
void prepareLinearSystem (
            int ntry,
            int nnewt )  [virtual]
```

Writes the Jacobian for the Newton iteration and passes it to the linear solver

Parameters

ntry	integer newton_try integer start number of Newton solver (1 or 2)
nnewt	integer number of current Newton step

Writes the Jacobian for the Newton iteration and passes it to the linear solver. Also wraps around getSensis for iterative linear solver.

Parameters

ntry	integer newton_try integer start number of Newton solver (1 or 2)
nnewt	integer number of current Newton step

Implements NewtonSolver.

Definition at line 329 of file newton_solver.cpp.

10.17.3.3 linsolveSPBCG()

```
void linsolveSPBCG (
            int ntry,
            int nnewt,
            AmiVector * ns_delta )
```

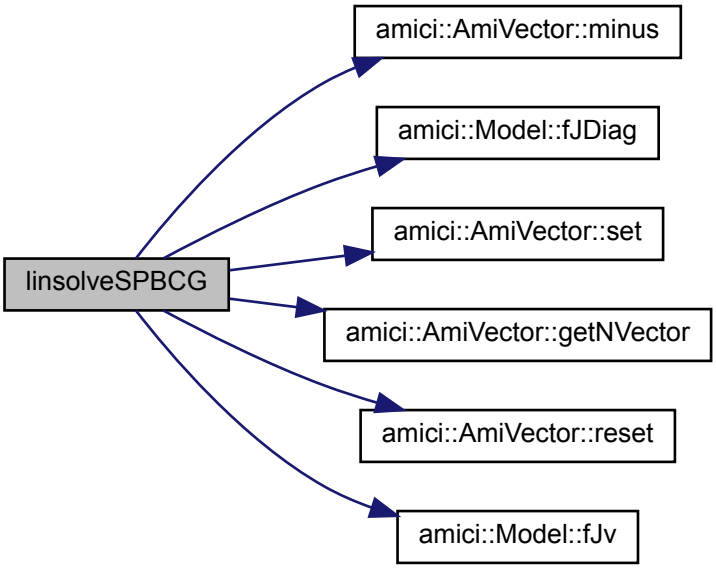
Iterative linear solver created from SPILS BiCG-Stab. Solves the linear system within each Newton step if iterative solver is chosen.

Parameters

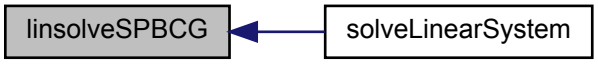
ntry	integer newton_try integer start number of Newton solver (1 or 2)
nnewt	integer number of current Newton step
ns_delta	Newton step

Definition at line 363 of file newton_solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

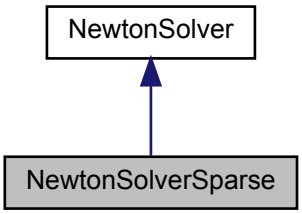


10.18 NewtonSolverSparse Class Reference

The NewtonSolverSparse provides access to the sparse linear solver for the Newton method.

```
#include <newton_solver.h>
```

Inheritance diagram for NewtonSolverSparse:



Public Member Functions

- NewtonSolverSparse (realtype ∗t, AmiVector ∗x, Model ∗model, ReturnData ∗rdata)
- void solveLinearSystem (AmiVector ∗rhs) override
- void prepareLinearSystem (int ntry, int nnewt) override

Additional Inherited Members

10.18.1 Detailed Description

Definition at line 109 of file newton_solver.h.

10.18.2 Constructor & Destructor Documentation

10.18.2.1 NewtonSolverSparse()

```
NewtonSolverSparse (
            realtype * t,
            AmiVector * x,
            Model * model,
            ReturnData * rdata )
```

default constructor, initializes all members with the provided objects, initializes temporary storage objects and the klu solver

Parameters

t	pointer to time variable
x	pointer to state variables
model	pointer to the AMICI model object
rdata	pointer to the return data object

Definition at line 221 of file newton_solver.cpp.

10.18.3 Member Function Documentation

10.18.3.1 solveLinearSystem()

```
void solveLinearSystem (
            AmiVector * rhs )  [override], [virtual]
```

Solves the linear system for the Newton step

Parameters

rhs	containing the RHS of the linear system, will be overwritten by solution to the linear system

Solves the linear system for the Newton step

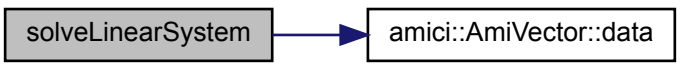
Parameters

rhs	containing the RHS of the linear system,will be overwritten by solution to the linear system

Implements NewtonSolver.

Definition at line 278 of file newton_solver.cpp.

Here is the call graph for this function:



10.18.3.2 prepareLinearSystem()

```
void prepareLinearSystem (
            int ntry,
            int nnewt )  [override], [virtual]
```

Writes the Jacobian for the Newton iteration and passes it to the linear solver

Parameters

ntry	integer newton_try integer start number of Newton solver (1 or 2)
nnewt	integer number of current Newton step

Writes the Jacobian for the Newton iteration and passes it to the linear solver

Parameters

ntry	integer newton_try integer start number of Newton solver (1 or 2)
nnewt	integer number of current Newton step

Implements NewtonSolver.

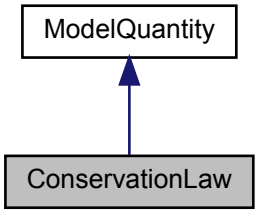
Definition at line 244 of file newton_solver.cpp.

Here is the call graph for this function:

10.19 ConservationLaw Class Reference

A conservation law defines the absolute the total amount of a (weighted) sum of states.

Inheritance diagram for ConservationLaw:



Public Member Functions

- def __init__ (self, identifier, name, value)

  Create a new ConservationLaw instance.

10.19.1 Detailed Description

Definition at line 497 of file ode_export.py.

10.19.2 Constructor & Destructor Documentation

10.19.2.1 __init__()

```
def __init__ (
            self,
            identifier,
            name,
            value )
```

Parameters

identifier	unique identifier of the ConservationLaw **Type**: sympy.Symbol
name	individual name of the ConservationLaw (does not need to be unique) **Type**: str
value	formula (sum of states) **Type**: symengine.Basic

Returns

ModelQuantity instance

TypeError

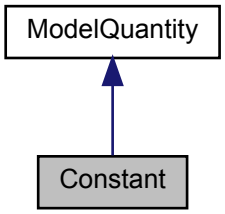
is thrown if input types do not match documented types

Definition at line 516 of file ode_export.py.

10.20 Constant Class Reference

A Constant is a fixed variable in the model with respect to which sensitivites cannot be computed, abbreviated by `k`

Inheritance diagram for Constant:



Public Member Functions

- def __init__ (self, identifier, name, value)

  Create a new Expression instance.

10.20.1 Detailed Description

Definition at line 632 of file ode_export.py.

10.20.2 Constructor & Destructor Documentation

10.20.2.1 __init__()

```
def __init__ (
            self,
            identifier,
            name,
            value )
```

Parameters

identifier	unique identifier of the Constant **Type**: sympy.Symbol
name	individual name of the Constant (does not need to be unique) **Type**: str
value	numeric value **Type**: float

Returns

ModelQuantity instance

TypeError

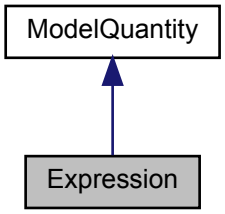
is thrown if input types do not match documented types

Definition at line 651 of file ode_export.py.

10.21 Expression Class Reference

An Expressions is a recurring elements in symbolic formulas.

Inheritance diagram for Expression:



Public Member Functions

- def __init__ (self, identifier, name, value)

  Create a new Expression instance.

10.21.1 Detailed Description

Specifying this may yield more compact expression which may lead to substantially shorter model compilation times, but may also reduce model simulation time, abbreviated by `w`

Definition at line 579 of file ode_export.py.

10.21.2 Constructor & Destructor Documentation

10.21.2.1 __init__()

```
def __init__ (
              self,
              identifier,
              name,
              value )
```

Parameters

identifier	unique identifier of the Expression **Type**: sympy.Symbol
name	individual name of the Expression (does not need to be unique) **Type**: str
value	formula **Type**: symengine.Basic

Returns

ModelQuantity instance

TypeError

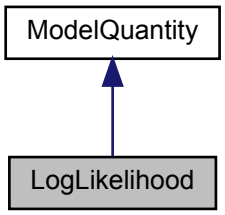
is thrown if input types do not match documented types

Definition at line 597 of file ode_export.py.

10.22 LogLikelihood Class Reference

A LogLikelihood defines the distance between measurements and experiments for a particular observable.

Inheritance diagram for LogLikelihood:



Public Member Functions

- def __init__ (self, identifier, name, value)

  Create a new Expression instance.

10.22.1 Detailed Description

The final LogLikelihood value in the simulation will be the sum of all specified LogLikelihood instances evaluated at all timepoints, abbreviated by `Jy`

Definition at line 661 of file ode_export.py.

10.22.2 Constructor & Destructor Documentation

10.22.2.1 __init__()

```
def __init__ (
              self,
              identifier,
              name,
              value )
```

Parameters

identifier	unique identifier of the LogLikelihood **Type**: sympy.Symbol
name	individual name of the LogLikelihood (does not need to be unique) **Type**: str
value	formula **Type**: symengine.Basic

Returns

ModelQuantity instance

TypeError

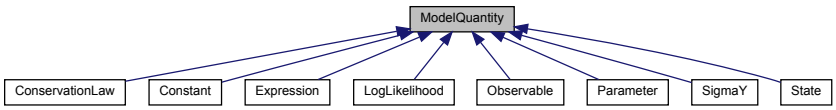
is thrown if input types do not match documented types

Definition at line 681 of file ode_export.py.

10.23 ModelQuantity Class Reference

Base class for model components.

Inheritance diagram for ModelQuantity:



Public Member Functions

- def __init__ (self, identifier, name, value)

  Create a new ModelQuantity instance.
- def __repr__ (self)

  Representation of the ModelQuantity object.
- def get_id (self)

  ModelQuantity identifier.
- def get_name (self)

  ModelQuantity name.
- def get_val (self)

  ModelQuantity value.

10.23.1 Detailed Description

Definition at line 299 of file ode_export.py.

10.23.2 Constructor & Destructor Documentation

10.23.2.1 __init__()

```
def __init__ (
            self,
            identifier,
            name,
            value )
```

This function sanitizes input from pysb to make sure we are operating on flat symby.Symbol and sympy.Basic and not respective derived pysb classes

Parameters

identifier	unique identifier of the quantity **Type**: sympy.Symbol
name	individual name of the quantity (does not need to be unique) **Type**: str
value	either formula, numeric value or initial value

Returns

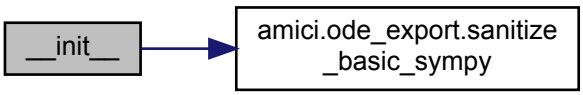
ModelQuantity instance

TypeError

is thrown if input types do not match documented types

Definition at line 319 of file ode_export.py.

Here is the call graph for this function:



10.23.3 Member Function Documentation

10.23.3.1 __repr__()

```
def __repr__ (
              self )
```

Returns

string representation of the ModelQuantity

Definition at line 357 of file ode_export.py.

10.23.3.2 get_id()

```
def get_id (
              self )
```

Returns

identifier of the ModelQuantity

Definition at line 370 of file ode_export.py.

10.23.3.3 get_name()

```
def get_name (
              self )
```

Returns

name of the ModelQuantity

Definition at line 383 of file ode_export.py.

10.23.3.4 get_val()

```
def get_val (
            self )
```

Returns

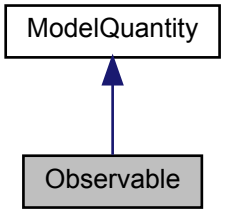
value of the ModelQuantity

Definition at line 396 of file ode_export.py.

10.24 Observable Class Reference

An Observable links model simulations to experimental measurements, abbreviated by `y`

Inheritance diagram for Observable:



Public Member Functions

- def __init__ (self, identifier, name, value)
  Create a new Observable instance.

10.24.1 Detailed Description

Definition at line 524 of file ode_export.py.

10.24.2 Constructor & Destructor Documentation

10.24.2.1 __init__()

```
def __init__ (
            self,
            identifier,
            name,
            value )
```

Parameters

identifier	unique identifier of the Observable **Type**: sympy.Symbol
name	individual name of the Observable (does not need to be unique) **Type**: str
value	formula **Type**: symengine.Basic

Returns

ModelQuantity instance

TypeError

is thrown if input types do not match documented types

Definition at line 542 of file ode_export.py.

10.25 ODEExporter Class Reference

The ODEExporter class generates AMICI C++ files for ODE model as defined in symbolic expressions.

Public Member Functions

- def __init__ (self, ode_model, outdir=None, verbose=False, assume_pow_positivity=False, compiler=None, allow_reinit_fixpar_initcond=True)

  Generate AMICI C++ files for the ODE provided to the constructor.
- def generateModelCode (self)

  Generates the native C++ code for the loaded model.
- def compileModel (self)

  Compiles the generated code it into a simulatable module.
- def setPaths (self, output_dir)

  Set output paths for the model and create if necessary.
- def setName (self, modelName)

  Sets the model name.

Public Attributes

- outdir

  see sbml_import.setPaths()
  ***Type**: str*
- verbose

  more verbose output if True
  ***Type**: bool*
- assume_pow_positivity

  if set to true, a special pow function is
- compiler

  distutils/setuptools compiler selection to build the

- modelName

  name of the model that will be used for compilation
- modelPath

  path to the generated model specific files
  ***Type**: str*
- modelSwigPath

  path to the generated swig files
  ***Type**: str*
- model

  ODE definition
  ***Type**: ODEModel.*
- functions

  carries C++ function signatures and other specifications
- allow_reinit_fixpar_initcond

  indicates whether reinitialization of

10.25.1 Detailed Description

initial states depending on fixedParmeters is allowed for this model
Type: bool

Definition at line 1859 of file ode_export.py.

10.25.2 Constructor & Destructor Documentation

10.25.2.1 __init__()

```
def __init__ (
              self,
              ode_model,
              outdir = None,
              verbose = False,
              assume_pow_positivity = False,
              compiler = None,
              allow_reinit_fixpar_initcond = True )
```

Parameters

ode_model	ODE definition **Type**: ODEModel
outdir	see sbml_import.setPaths() **Type**: str
verbose	more verbose output if True **Type**: bool
assume_pow_positivity	if set to true, a special pow function is used to avoid problems with state variables that may become negative due to numerical errors **Type**: bool
compiler	distutils/setuptools compiler selection to build the python extension **Type**: str
allow_reinit_fixpar_initcond	see ODEExporter

Returns

Definition at line 1949 of file ode_export.py.

10.25.3 Member Function Documentation

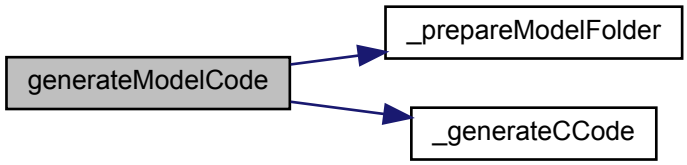
10.25.3.1 generateModelCode()

```
def generateModelCode (
              self )
```

Returns

Definition at line 1981 of file ode_export.py.

Here is the call graph for this function:



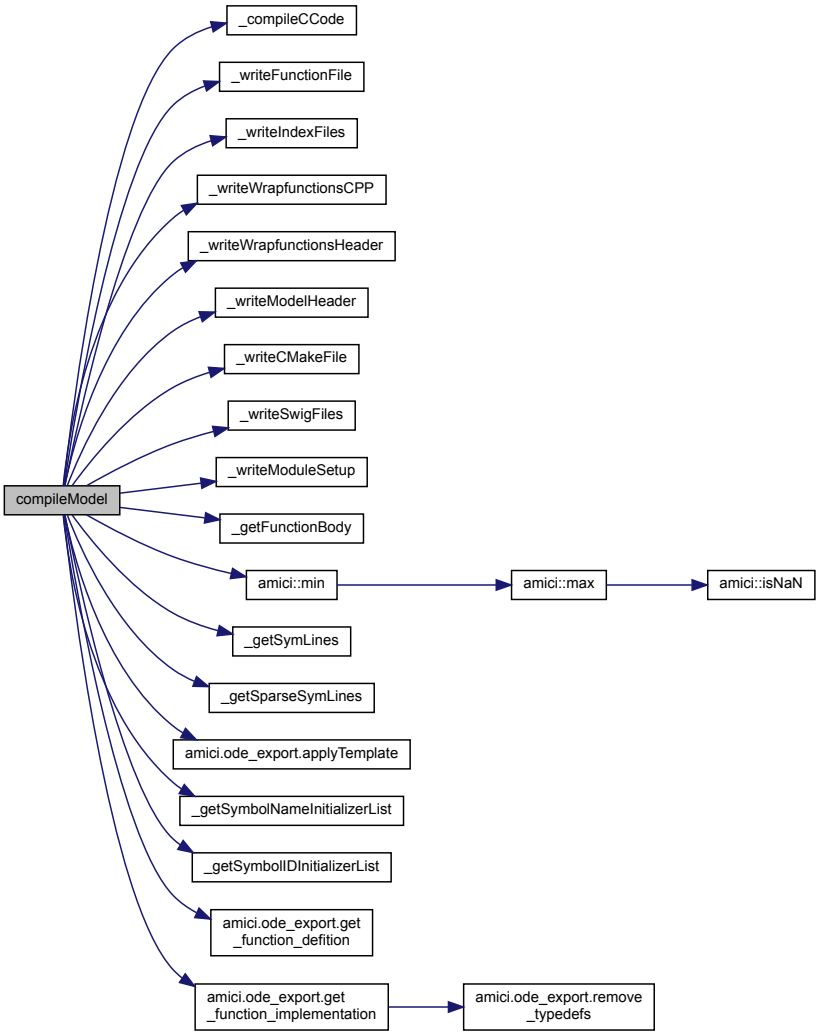
10.25.3.2 compileModel()

```
def compileModel (
              self )
```

Returns

Definition at line 1994 of file ode_export.py.

Here is the call graph for this function:



10.25.3.3 setPaths()

```
def setPaths (
            self,
            output_dir )
```

Parameters

output_dir	relative or absolute path where the generated model code is to be placed. will be created if does not exists. **Type**: str

Returns

Definition at line 2600 of file ode_export.py.

10.25.3.4 setName()

```
def setName (
            self,
            modelName )
```

Parameters

modelName	name of the model (must only contain valid filename characters) **Type**: str

Returns

Definition at line 2619 of file ode_export.py.

10.26 ODEModel Class Reference

An ODEModel defines an Ordinay Differential Equation as set of ModelQuantities.

Public Member Functions

- def __init__ (self)

  Create a new ODEModel instance.
- def import_from_sbml_importer (self, si)

  Imports a model specification from a amici.SBMLImporter instance.
- def add_component (self, component)

  Adds a new ModelQuantity to the model.
- def add_conservation_law (self, state, law)

  Adds a new conservation law to the model.
- def nx_rdata (self)

  Number of states.
- def nx_solver (self)

Number of states after applying conservation laws.

- def ncl (self)

  Number of conservation laws.
- def ny (self)

  Number of Observables.
- def nk (self)

  Number of Constants.
- def np (self)

  Number of Parameters.
- def sym (self, name)

  Returns (and constructs if necessary) the identifiers for a symbolic entity.
- def sparsesym (self, name)

  Returns (and constructs if necessary) the sparsified identifiers for a sparsified symbolic variable.
- def eq (self, name)

  Returns (and constructs if necessary) the formulas for a symbolic entity.
- def sparseeq (self, name)

  Returns (and constructs if necessary) the sparsified formulas for a sparsified symbolic variable.
- def colptr (self, name)

  Returns (and constructs if necessary) the column pointers for a sparsified symbolic variable.
- def rowval (self, name)

  Returns (and constructs if necessary) the row values for a sparsified symbolic variable.
- def val (self, name)

  Returns (and constructs if necessary) the numeric values of a symbolic entity.
- def name (self, name)

  Returns (and constructs if necessary) the names of a symbolic variable.
- def generateBasicVariables (self)

  Generates the symbolic identifiers for all variables in ODEModel.variable_prototype.
- def symNames (self)

  Returns a list of names of generated symbolic variables.
- def sym_or_eq (self, name, varname)

  Returns symbols or equations depending on whether a given variable appears in the function signature or not.
- def get_conservation_laws (self)

  Returns a list of states with conservation law set.
- def state_has_fixed_parameter_initial_condition (self, ix)

  Checks whether the state at specified index has a fixed parameter initial condition.
- def state_has_conservation_law (self, ix)

  Checks whether the state at specified index has a conservation law set.

10.26.1 Detailed Description

This class provides general purpose interfaces to compute arbitrary symbolic derivatives that are necessary for model simulation or sensitivity computation

```
derivative from a partial derivative call to enforce a partial
derivative in the next recursion. prevents infinite recursion
```

Definition at line 707 of file ode_export.py.

10.26.2 Constructor & Destructor Documentation

10.26.2.1 __init__()

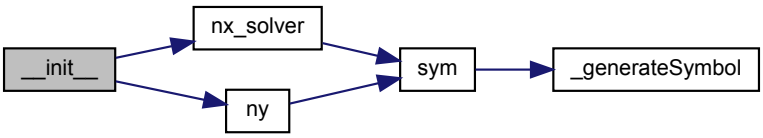
```
def __init__ (
              self )
```

Returns

New ODEModel instance

Definition at line 867 of file ode_export.py.

Here is the call graph for this function:



10.26.3 Member Function Documentation

10.26.3.1 import_from_sbml_importer()

```
def import_from_sbml_importer (
              self,
              si )
```

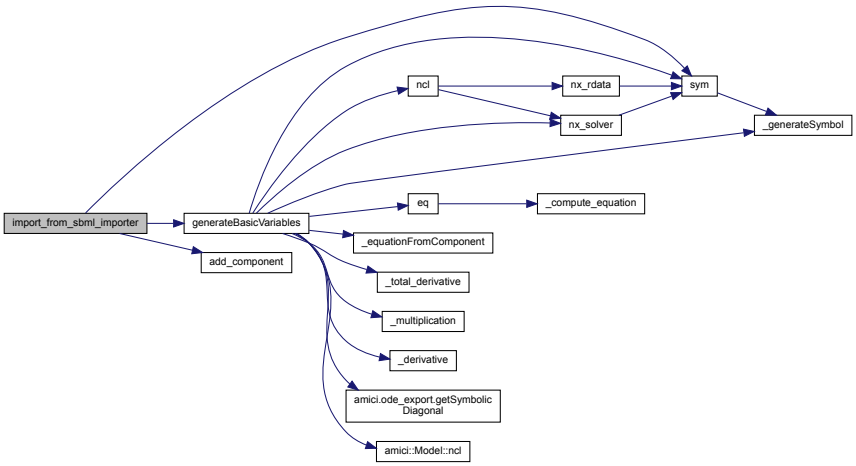
Parameters

si	imported SBML model **Type**: amici.SbmlImporter

Returns

Definition at line 969 of file ode_export.py.

Here is the call graph for this function:



10.26.3.2 add_component()

```
def add_component (
            self,
            component )
```

Parameters

component	model quantity to be added **Type**: ModelQuantity

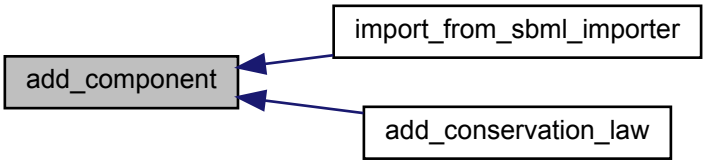
Returns

Exceptions

Exception	invalid component type

Definition at line 1003 of file ode_export.py.

Here is the caller graph for this function:



10.26.3.3 add_conservation_law()

```
def add_conservation_law (
              self,
              state,
              law )
```

Parameters

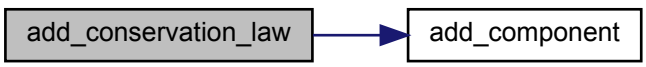
state	symbolic identifier of the state that should be replaced by the conservation law
law	symbolic formula that together with the state defines the conservation law, i.e., d/dt (state + law) = 0

Returns

```
Exception if the specified state does not correspond to a valid
state in the model
```

Definition at line 1028 of file ode_export.py.

Here is the call graph for this function:



10.26.3.4 nx_rdata()

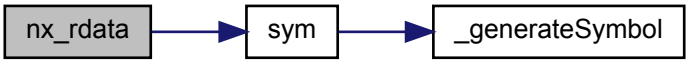
```
def nx_rdata (
              self )
```

Returns

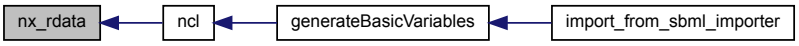
number of state variable symbols

Definition at line 1072 of file ode_export.py.

Here is the call graph for this function:



Here is the caller graph for this function:



10.26.3.5 nx_solver()

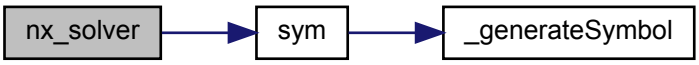
```
def nx_solver (
              self )
```

Returns

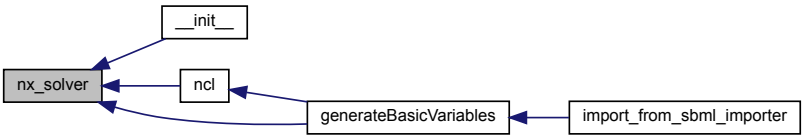
number of state variable symbols

Definition at line 1085 of file ode_export.py.

Here is the call graph for this function:



Here is the caller graph for this function:



10.26.3.6 ncl()

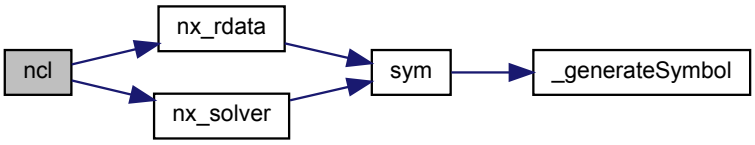
```
def ncl (
            self )
```

Returns

number of state variable symbols

Definition at line 1098 of file ode_export.py.

Here is the call graph for this function:



Here is the caller graph for this function:

10.26.3.7 ny()

```
def ny (
            self )
```

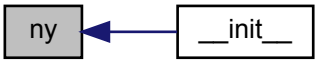
Returns

number of observable symbols

Definition at line 1111 of file ode_export.py.

Here is the call graph for this function:

Here is the caller graph for this function:



10.26.3.8 nk()

```
def nk (
            self )
```

Returns

number of constant symbols

Definition at line 1124 of file ode_export.py.

Here is the call graph for this function:

10.26.3.9 np()

```
def np (
            self )
```

Returns

number of parameter symbols

Definition at line 1137 of file ode_export.py.

Here is the call graph for this function:

10.26.3.10 sym()

```
def sym (
            self,
            name )
```

Parameters

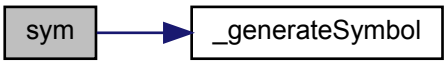
name	name of the symbolic variable **Type**: str

Returns

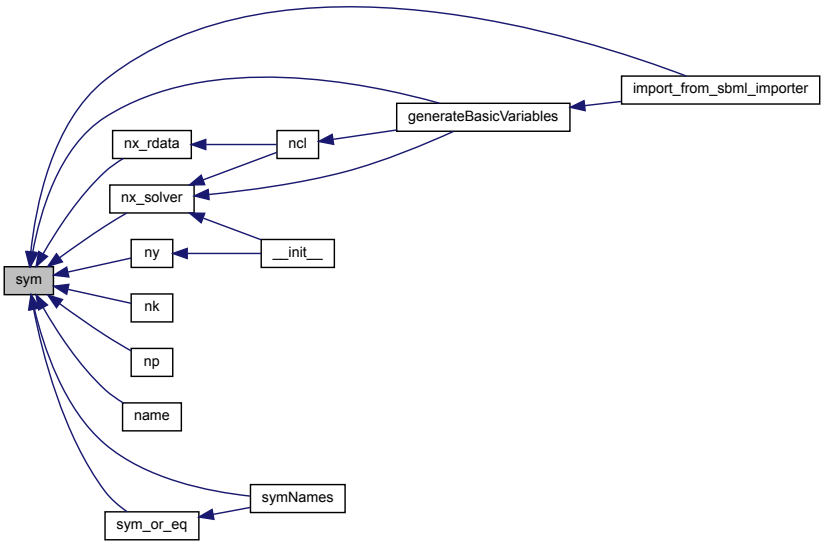
containing the symbolic identifiers
Type: symengine.DenseMatrix

Definition at line 1152 of file ode_export.py.

Here is the call graph for this function:



Here is the caller graph for this function:



10.26.3.11 sparsesym()

```
def sparsesym (
            self,
            name )
```

Parameters

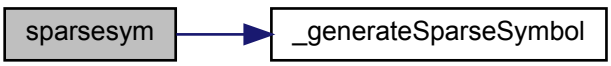
name	name of the symbolic variable **Type**: str

Returns

linearized symengine.DenseMatrix containing the symbolic identifiers

Definition at line 1169 of file ode_export.py.

Here is the call graph for this function:



10.26.3.12 eq()

```
def eq (
            self,
            name )
```

Parameters

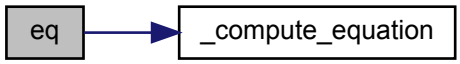
name	name of the symbolic variable **Type**: str

Returns

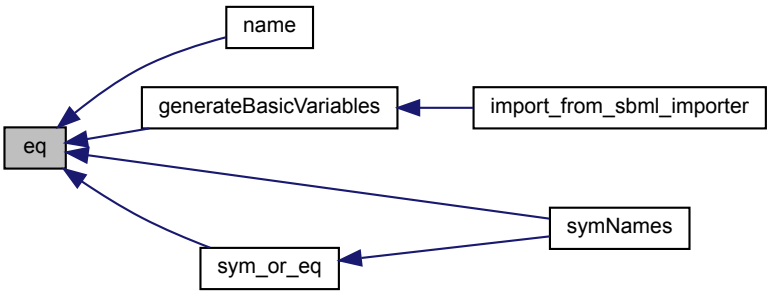
symengine.DenseMatrix containing the symbolic identifiers

Definition at line 1188 of file ode_export.py.

Here is the call graph for this function:



Here is the caller graph for this function:



10.26.3.13 sparseeq()

```
def sparseeq (
            self,
            name )
```

Parameters

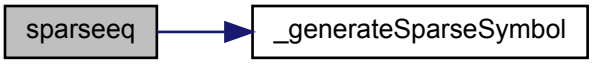
name	name of the symbolic variable **Type**: str

Returns

linearized symengine.DenseMatrix containing the symbolic formulas

Definition at line 1206 of file ode_export.py.

Here is the call graph for this function:



10.26.3.14 colptr()

```
def colptr (
            self,
            name )
```

Parameters

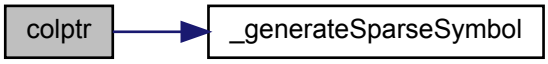
name	name of the symbolic variable **Type**: str

Returns

symengine.DenseMatrix containing the column pointers

Definition at line 1225 of file ode_export.py.

Here is the call graph for this function:



10.26.3.15 rowval()

```
def rowval (
            self,
            name )
```

Parameters

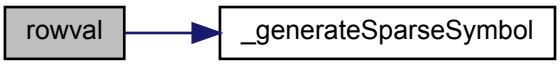
name	name of the symbolic variable **Type**: str

Returns

symengine.DenseMatrix containing the row values

Definition at line 1244 of file ode_export.py.

Here is the call graph for this function:



10.26.3.16 val()

```
def val (
            self,
            name )
```

Parameters

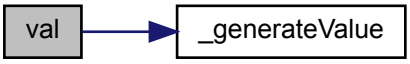
name	name of the symbolic variable **Type**: str

Returns

list containing the numeric values

Definition at line 1263 of file ode_export.py.

Here is the call graph for this function:



10.26.3.17 name()

```
def name (
            self,
            name )
```

Parameters

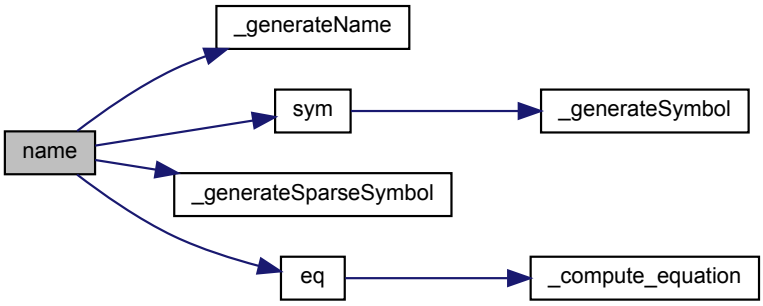
name	name of the symbolic variable **Type**: str

Returns

list of names

Definition at line 1280 of file ode_export.py.

Here is the call graph for this function:



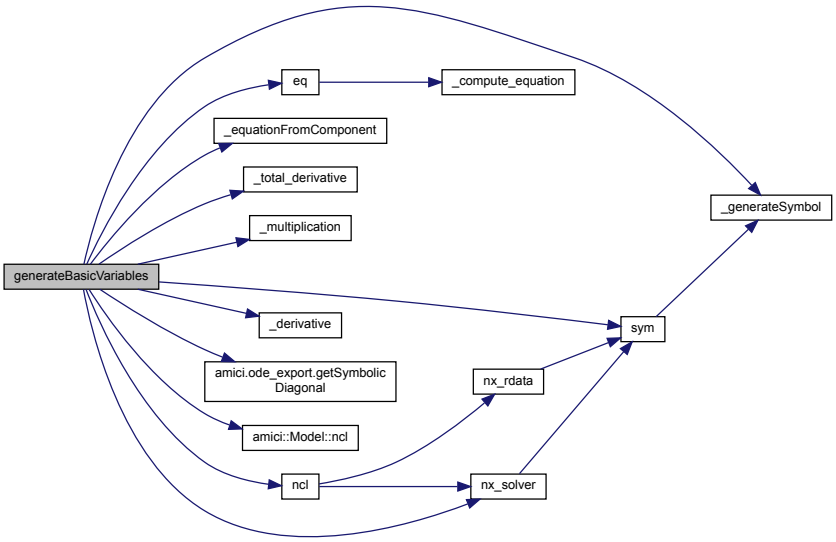
10.26.3.18 generateBasicVariables()

```
def generateBasicVariables (
            self )
```

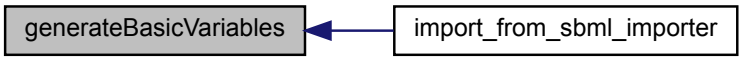
Returns

Definition at line 1350 of file ode_export.py.

Here is the call graph for this function:



Here is the caller graph for this function:



10.26.3.19 symNames()

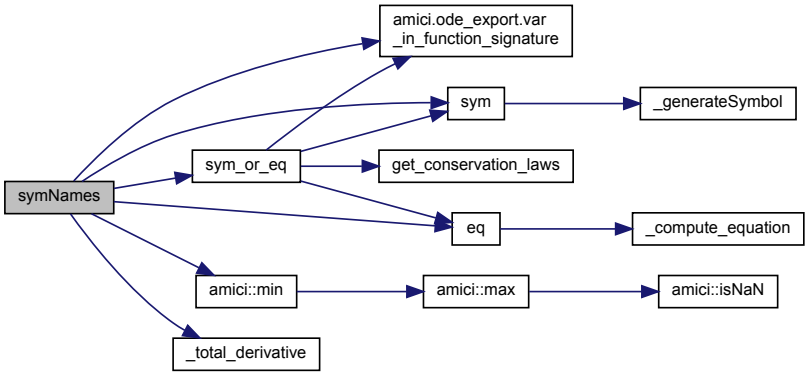
```
def symNames (
            self )
```

Returns

list of names

Definition at line 1544 of file ode_export.py.

Here is the call graph for this function:



10.26.3.20 sym_or_eq()

```
def sym_or_eq (
              self,
              name,
              varname )
```

Parameters

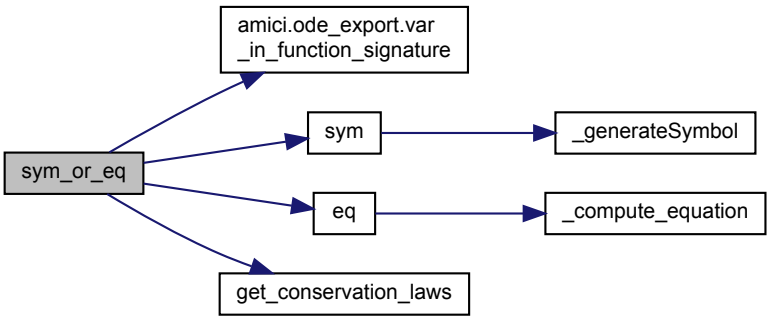
name	name of function for which the signature should be checked
varname	name of the variable which should be contained in the function signature

Returns

the variable symbols if the variable is part of the signature and the variable equations otherwise.

Definition at line 1673 of file ode_export.py.

Here is the call graph for this function:



Here is the caller graph for this function:

10.26.3.21 get_conservation_laws()

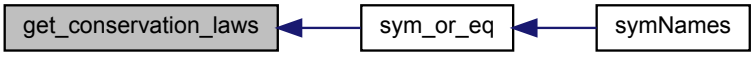
```
def get_conservation_laws (
                self )
```

Returns

list of state identifiers

Definition at line 1757 of file ode_export.py.

Here is the caller graph for this function:



10.26.3.22 state_has_fixed_parameter_initial_condition()

```
def state_has_fixed_parameter_initial_condition (
              self,
              ix )
```

Parameters

ix	state index

Returns

boolean indicating if any of the initial condition free variables is contained in the model constants

Definition at line 1826 of file ode_export.py.

10.26.3.23 state_has_conservation_law()

```
def state_has_conservation_law (
              self,
              ix )
```

Parameters

ix	state index

Returns

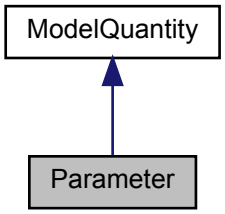
boolean indicating if conservation_law is not None

Definition at line 1847 of file ode_export.py.

10.27 Parameter Class Reference

A Parameter is a free variable in the model with respect to which sensitivites may be computed, abbreviated by `p`

Inheritance diagram for Parameter:



Public Member Functions

- def __init__ (self, identifier, name, value)

  Create a new Expression instance.

10.27.1 Detailed Description

Definition at line 605 of file ode_export.py.

10.27.2 Constructor & Destructor Documentation

10.27.2.1 __init__()

```
def __init__ (
            self,
            identifier,
            name,
            value )
```

Parameters

identifier	unique identifier of the Parameter **Type**: sympy.Symbol
name	individual name of the Parameter (does not need to be unique) **Type**: str
value	numeric value **Type**: float

Returns

ModelQuantity instance

TypeError

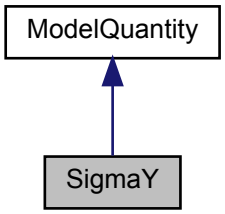
is thrown if input types do not match documented types

Definition at line 624 of file ode_export.py.

10.28 SigmaY Class Reference

A Standard Deviation SigmaY rescales the distance between simulations and measurements when computing residuals, abbreviated by `sigmay`

Inheritance diagram for SigmaY:



Public Member Functions

- def __init__ (self, identifier, name, value)

  Create a new Standard Deviation instance.

10.28.1 Detailed Description

Definition at line 550 of file ode_export.py.

10.28.2 Constructor & Destructor Documentation

10.28.2.1 __init__()

```
def __init__ (
              self,
              identifier,
              name,
              value )
```

Parameters

identifier	unique identifier of the Standard Deviation **Type**: sympy.Symbol
name	individual name of the Standard Deviation (does not need to be unique) **Type**: str
value	formula **Type**: symengine.Basic

Returns

ModelQuantity instance

TypeError

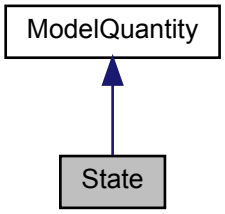
is thrown if input types do not match documented types

Definition at line 569 of file ode_export.py.

10.29 State Class Reference

A State variable defines an entity that evolves with time according to the provided time derivative, abbreviated by `x`

Inheritance diagram for State:



Public Member Functions

- def __init__ (self, identifier, name, value, dt)

  Create a new State instance.
- def set_conservation_law (self, law)

  Sets the conservation law of a state.
- def set_dt (self, dt)

  Sets the time derivative.
- def get_dt (self)

  Sets the time derivative.

Static Public Attributes

- conservation_law = None

  algebraic formula that allows computation of this

10.29.1 Detailed Description

species according to a conservation law

Definition at line 407 of file ode_export.py.

10.29.2 Constructor & Destructor Documentation

10.29.2.1 __init__()

```
def __init__ (
              self,
              identifier,
              name,
              value,
              dt )
```

Extends ModelQuantity.__init__ by dt

Parameters

identifier	unique identifier of the state **Type**: sympy.Symbol
name	individual name of the state (does not need to be unique) **Type**: str
value	initial value **Type**: symengine.Basic
dt	time derivative **Type**: symengine.Basic

Returns

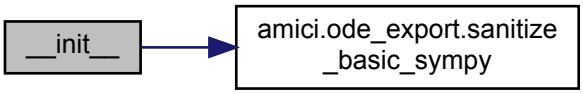
ModelQuantity instance

TypeError

is thrown if input types do not match documented types

Definition at line 433 of file ode_export.py.

Here is the call graph for this function:



10.29.3 Member Function Documentation

10.29.3.1 set_conservation_law()

```
def set_conservation_law (
              self,
              law )
```

If the a conservation law is set, the respective state will be replaced by an algebraic formula according to the respective conservation law.

Parameters

law	linear sum of states that if added to this state remain constant over time

Returns

TypeError

is thrown if law type does not match documented type

Definition at line 456 of file ode_export.py.

10.29.3.2 set_dt()

```
def set_dt (
              self,
              dt )
```

Parameters

dt	time derivative **Type**: symengine.Basic

Returns

TypeError

is thrown if dt type does not match documented type

Definition at line 474 of file ode_export.py.

10.29.3.3 get_dt()

```
def get_dt (
            self )
```

Returns

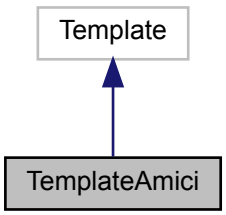
time derivative
Type: symengine.Basic

Definition at line 489 of file ode_export.py.

10.30 TemplateAmici Class Reference

Template format used in AMICI (see string.template for more details).

Inheritance diagram for TemplateAmici:



Static Public Attributes

- string delimiter = 'TPL_'

  delimiter that identifies template variables
  ***Type**: str*

10.30.1 Detailed Description

Definition at line 2647 of file ode_export.py.

10.31 ReturnData Class Reference

class that stores all data which is later returned by the mex function

```
#include <rdata.h>
```

Public Member Functions

- ReturnData ()

  default constructor
- ReturnData (std::vector< realtype > ts, int np, int nk, int nx, int nx_solver, int nxtrue, int ny, int nytrue, int nz, int nztrue, int ne, int nJ, int nplist, int nmaxevent, int nt, int newton_maxsteps, std::vector< ParameterScaling > pscale, SecondOrderMode o2mode, SensitivityOrder sensi, SensitivityMethod sensi_meth)

  ReturnData.
- ReturnData (Solver const &solver, const Model *model)
- void initializeObjectiveFunction ()

  initializeObjectiveFunction
- void invalidate (const realtype t)
- void invalidateLLH ()
- void applyChainRuleFactorToSimulationResults (const Model *model)

Public Attributes

- const std::vector< realtype > ts
- std::vector< realtype > xdot
- std::vector< realtype > J
- std::vector< realtype > z
- std::vector< realtype > sigmaz
- std::vector< realtype > sz
- std::vector< realtype > ssigmaz
- std::vector< realtype > rz
- std::vector< realtype > srz
- std::vector< realtype > s2rz
- std::vector< realtype > x
- std::vector< realtype > sx
- std::vector< realtype > y
- std::vector< realtype > sigmay
- std::vector< realtype > sy
- std::vector< realtype > ssigmay
- std::vector< realtype > res
- std::vector< realtype > sres
- std::vector< realtype > FIM
- std::vector< int > numsteps
- std::vector< int > numstepsB
- std::vector< int > numrhsevals
- std::vector< int > numrhsevalsB
- std::vector< int > numerrtestfails

- std::vector< int > numerrtestfailsB
- std::vector< int > numnonlinsolvconvfails
- std::vector< int > numnonlinsolvconvfailsB
- std::vector< int > order
- int newton_status = 0
- double newton_cpu_time = 0.0
- std::vector< int > newton_numsteps
- std::vector< int > newton_numlinsteps
- realtype t_steadystate = NAN
- realtype wrms_steadystate = NAN
- realtype wrms_sensi_steadystate = NAN
- std::vector< realtype > x0
- std::vector< realtype > sx0
- realtype llh = 0.0
- realtype chi2 = 0.0
- std::vector< realtype > sllh
- std::vector< realtype > s2llh
- int status = 0
- const int np
- const int nk
- const int nx
- const int nx_solver
- const int nxtrue
- const int ny
- const int nytrue
- const int nz
- const int nztrue
- const int ne
- const int nJ
- const int nplist
- const int nmaxevent
- const int nt
- const int newton_maxsteps
- std::vector< ParameterScaling > pscale
- const SecondOrderMode o2mode
- const SensitivityOrder sensi
- const SensitivityMethod sensi_meth

Friends

- template<class Archive >
  void boost::serialization::serialize (Archive &ar, ReturnData &r, const unsigned int version)

  Serialize ReturnData (see boost::serialization::serialize)

10.31.1 Detailed Description

NOTE: multidimensional arrays are stored in row-major order (FORTRAN-style)

Definition at line 28 of file rdata.h.

10.31.2 Constructor & Destructor Documentation

10.31.2.1 ReturnData() [1/2]

```
ReturnData (
            std::vector< realtype > ts,
            int np,
            int nk,
            int nx,
            int nx_solver,
            int nxtrue,
            int ny,
            int nytrue,
            int nz,
            int nztrue,
            int ne,
            int nJ,
            int nplist,
            int nmaxevent,
            int nt,
            int newton_maxsteps,
            std::vector< ParameterScaling > pscale,
            SecondOrderMode o2mode,
            SensitivityOrder sensi,
            SensitivityMethod sensi_meth )
```

Parameters

ts	see amici::Model::ts
np	see amici::Model::np
nk	see amici::Model::nk
nx	see amici::Model::nx_rdata
nx_solver	see amici::Model::nx_solver
nxtrue	see amici::Model::nxtrue_rdata
ny	see amici::Model::ny
nytrue	see amici::Model::nytrue
nz	see amici::Model::nz
nztrue	see amici::Model::nztrue
ne	see amici::Model::ne
nJ	see amici::Model::nJ
nplist	see amici::Model::nplist
nmaxevent	see amici::Model::nmaxevent
nt	see amici::Model::nt
newton_maxsteps	see amici::Solver::newton_maxsteps
pscale	see amici::Model::pscale
o2mode	see amici::Model::o2mode
sensi	see amici::Solver::sensi
sensi_meth	see amici::Solver::sensi_meth

Definition at line 40 of file rdata.cpp.

Here is the call graph for this function:

10.31.2.2 ReturnData() [2/2]

```
ReturnData (
            Solver const & solver,
            const Model * model )
```

constructor that uses information from model and solver to appropriately initialize fields

Parameters

solver	solver
model	pointer to model specification object bool

Definition at line 22 of file rdata.cpp.

10.31.3 Member Function Documentation

10.31.3.1 invalidate()

```
void invalidate (
            const realtype t )
```

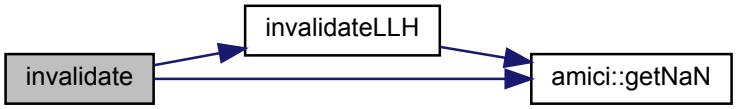
routine to set likelihood, state variables, outputs and respective sensitivities to NaN (typically after integration failure)

Parameters

t	time of integration failure

Definition at line 117 of file rdata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.31.3.2 invalidateLLH()

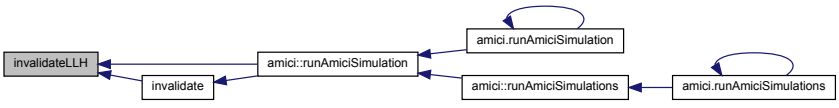
```
void invalidateLLH ( )
```

routine to set likelihood and respective sensitivities to NaN (typically after integration failure)

Definition at line 156 of file rdata.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



10.31.3.3 applyChainRuleFactorToSimulationResults()

```
void applyChainRuleFactorToSimulationResults (
            const Model * model )
```

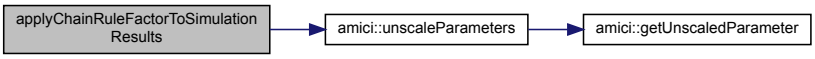
applies the chain rule to account for parameter transformation in the sensitivities of simulation results

Parameters

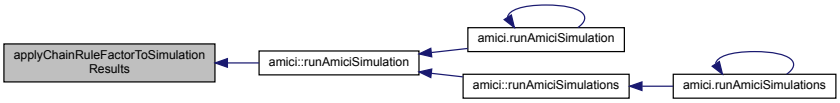
model	Model from which the ReturnData was obtained

Definition at line 168 of file rdata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.31.4 Friends And Related Function Documentation

10.31.4.1 boost::serialization::serialize

```
void boost::serialization::serialize (
            Archive & ar,
            ReturnData & r,
            const unsigned int version )  [friend]
```

Parameters

ar	Archive to serialize to
r	Data to serialize
version	Version number

10.31.5 Member Data Documentation

10.31.5.1 ts

```
const std::vector<realtype> ts
```

timepoints (dimension: nt)

Definition at line 78 of file rdata.h.

10.31.5.2 xdot

```
std::vector<realtype> xdot
```

time derivative (dimension: nx)

Definition at line 81 of file rdata.h.

10.31.5.3 J

```
std::vector<realtype> J
```

Jacobian of differential equation right hand side (dimension: nx x nx, row-major)

Definition at line 85 of file rdata.h.

10.31.5.4 z

```
std::vector<realtype> z
```

event output (dimension: nmaxevent x nz, row-major)

Definition at line 88 of file rdata.h.

10.31.5.5 sigmaz

```
std::vector<realtype> sigmaz
```

event output sigma standard deviation (dimension: nmaxevent x nz, row-major)

Definition at line 92 of file rdata.h.

10.31.5.6 sz

```
std::vector<realtype> sz
```

parameter derivative of event output (dimension: nmaxevent x nz, row-major)

Definition at line 96 of file rdata.h.

10.31.5.7 ssigmaz

```
std::vector<realtype> ssigmaz
```

parameter derivative of event output standard deviation (dimension: nmaxevent x nz, row-major)

Definition at line 100 of file rdata.h.

10.31.5.8 rz

```
std::vector<realtype> rz
```

event trigger output (dimension: nmaxevent x nz, row-major)

Definition at line 103 of file rdata.h.

10.31.5.9 srz

```
std::vector<realtype> srz
```

parameter derivative of event trigger output (dimension: nmaxevent x nz x nplist, row-major)

Definition at line 107 of file rdata.h.

10.31.5.10 s2rz

```
std::vector<realtype> s2rz
```

second order parameter derivative of event trigger output (dimension: nmaxevent x nztrue x nplist x nplist, row-major)

Definition at line 111 of file rdata.h.

10.31.5.11 x

```
std::vector<realtype> x
```

state (dimension: nt x nx, row-major)

Definition at line 114 of file rdata.h.

10.31.5.12 sx

```
std::vector<realtype> sx
```

parameter derivative of state (dimension: nt x nplist x nx, row-major)

Definition at line 118 of file rdata.h.

10.31.5.13 y

```
std::vector<realtype> y
```

observable (dimension: nt x ny, row-major)

Definition at line 121 of file rdata.h.

10.31.5.14 sigmay

```
std::vector<realtype> sigmay
```

observable standard deviation (dimension: nt x ny, row-major)

Definition at line 124 of file rdata.h.

10.31.5.15 sy

```
std::vector<realtype> sy
```

parameter derivative of observable (dimension: nt x nplist x ny, row-major)

Definition at line 128 of file rdata.h.

10.31.5.16 ssigmay

```
std::vector<realtype> ssigmay
```

parameter derivative of observable standard deviation (dimension: nt x nplist x ny, row-major)

Definition at line 132 of file rdata.h.

10.31.5.17 res

```
std::vector<realtype> res
```

observable (dimension: nt∗ny, row-major)

Definition at line 135 of file rdata.h.

10.31.5.18 sres

```
std::vector<realtype> sres
```

parameter derivative of residual (dimension: nt∗ny x nplist, row-major)

Definition at line 139 of file rdata.h.

10.31.5.19 FIM

```
std::vector<realtype> FIM
```

fisher information matrix (dimension: nplist x nplist, row-major)

Definition at line 143 of file rdata.h.

10.31.5.20 numsteps

```
std::vector<int> numsteps
```

number of integration steps forward problem (dimension: nt)

Definition at line 146 of file rdata.h.

10.31.5.21 numstepsB

```
std::vector<int> numstepsB
```

number of integration steps backward problem (dimension: nt)

Definition at line 149 of file rdata.h.

10.31.5.22 numrhsevals

```
std::vector<int> numrhsevals
```

number of right hand side evaluations forward problem (dimension: nt)

Definition at line 152 of file rdata.h.

10.31.5.23 numrhsevalsB

```
std::vector<int> numrhsevalsB
```

number of right hand side evaluations backwad problem (dimension: nt)

Definition at line 155 of file rdata.h.

10.31.5.24 numerrtestfails

```
std::vector<int> numerrtestfails
```

number of error test failures forward problem (dimension: nt)

Definition at line 158 of file rdata.h.

10.31.5.25 numerrtestfailsB

```
std::vector<int> numerrtestfailsB
```

number of error test failures backwad problem (dimension: nt)

Definition at line 161 of file rdata.h.

10.31.5.26 numnonlinsolvconvfails

```
std::vector<int> numnonlinsolvconvfails
```

number of linear solver convergence failures forward problem (dimension: nt)

Definition at line 165 of file rdata.h.

10.31.5.27 numnonlinsolvconvfailsB

```
std::vector<int> numnonlinsolvconvfailsB
```

number of linear solver convergence failures backwad problem (dimension: nt)

Definition at line 169 of file rdata.h.

10.31.5.28 order

```
std::vector<int> order
```

employed order forward problem (dimension: nt)

Definition at line 172 of file rdata.h.

10.31.5.29 newton_status

```
int newton_status = 0
```

flag indicating success of Newton solver

Definition at line 175 of file rdata.h.

10.31.5.30 newton_cpu_time

```
double newton_cpu_time = 0.0
```

computation time of the Newton solver [s]

Definition at line 178 of file rdata.h.

10.31.5.31 newton_numsteps

```
std::vector<int> newton_numsteps
```

number of Newton steps for steady state problem (length = 2)

Definition at line 181 of file rdata.h.

10.31.5.32 newton_numlinsteps

```
std::vector<int> newton_numlinsteps
```

number of linear steps by Newton step for steady state problem (length = newton_maxsteps $*$ 2)

Definition at line 184 of file rdata.h.

10.31.5.33 t_steadystate

```
realtype t_steadystate = NAN
```

time at which steadystate was reached in the simulation based approach

Definition at line 187 of file rdata.h.

10.31.5.34 wrms_steadystate

```
realtype wrms_steadystate = NAN
```

weighted root-mean-square of the rhs when steadystate was reached

Definition at line 191 of file rdata.h.

10.31.5.35 wrms_sensi_steadystate

```
realtype wrms_sensi_steadystate = NAN
```

weighted root-mean-square of the rhs when steadystate was reached

Definition at line 195 of file rdata.h.

10.31.5.36 x0

```
std::vector<realtype> x0
```

preequilibration steady state found be Newton solver (dimension: nx)

Definition at line 198 of file rdata.h.

10.31.5.37 sx0

```
std::vector<realtype> sx0
```

preequilibration sensitivities found be Newton solver (dimension: nplist x nx, row-major)

Definition at line 201 of file rdata.h.

10.31.5.38 llh

```
realtype llh = 0.0
```

loglikelihood value

Definition at line 204 of file rdata.h.

10.31.5.39 chi2

```
realtype chi2 = 0.0
```

chi2 value

Definition at line 207 of file rdata.h.

10.31.5.40 sllh

```
std::vector<realtype> sllh
```

parameter derivative of loglikelihood (dimension: nplist)

Definition at line 210 of file rdata.h.

10.31.5.41 s2llh

```
std::vector<realtype> s2llh
```

second order parameter derivative of loglikelihood (dimension: (nJ-1) x nplist, row-major)

Definition at line 214 of file rdata.h.

10.31.5.42 status

```
int status = 0
```

status code

Definition at line 217 of file rdata.h.

10.31.5.43 np

```
const int np
```

total number of model parameters

Definition at line 220 of file rdata.h.

10.31.5.44 nk

```
const int nk
```

number of fixed parameters

Definition at line 222 of file rdata.h.

10.31.5.45 nx

```
const int nx
```

number of states

Definition at line 224 of file rdata.h.

10.31.5.46 nx_solver

```
const int nx_solver
```

number of observables with conservation laws applied

Definition at line 226 of file rdata.h.

10.31.5.47 nxtrue

```
const int nxtrue
```

number of states in the unaugmented system

Definition at line 228 of file rdata.h.

10.31.5.48 ny

```
const int ny
```

number of observables

Definition at line 230 of file rdata.h.

10.31.5.49 nytrue

```
const int nytrue
```

number of observables in the unaugmented system

Definition at line 232 of file rdata.h.

10.31.5.50 nz

```
const int nz
```

number of event outputs

Definition at line 234 of file rdata.h.

10.31.5.51 nztrue

```
const int nztrue
```

number of event outputs in the unaugmented system

Definition at line 236 of file rdata.h.

10.31.5.52 ne

```
const int ne
```

number of events

Definition at line 238 of file rdata.h.

10.31.5.53 nJ

```
const int nJ
```

dimension of the augmented objective function for 2nd order ASA

Definition at line 240 of file rdata.h.

10.31.5.54 nplist

```
const int nplist
```

number of parameter for which sensitivities were requested

Definition at line 243 of file rdata.h.

10.31.5.55 nmaxevent

```
const int nmaxevent
```

maximal number of occuring events (for every event type)

Definition at line 245 of file rdata.h.

10.31.5.56 nt

```
const int nt
```

number of considered timepoints

Definition at line 247 of file rdata.h.

10.31.5.57 newton_maxsteps

```
const int newton_maxsteps
```

maximal number of newton iterations for steady state calculation

Definition at line 249 of file rdata.h.

10.31.5.58 pscale

```
std::vector<ParameterScaling> pscale
```

scaling of parameterization (lin,log,log10)

Definition at line 251 of file rdata.h.

10.31.5.59 o2mode

```
const SecondOrderMode o2mode
```

flag indicating whether second order sensitivities were requested

Definition at line 253 of file rdata.h.

10.31.5.60 sensi

```
const SensitivityOrder sensi
```

sensitivity order

Definition at line 255 of file rdata.h.

10.31.5.61 sensi_meth

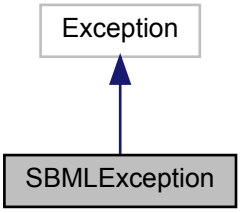
```
const SensitivityMethod sensi_meth
```

sensitivity method

Definition at line 257 of file rdata.h.

10.32 SBMLException Class Reference

Inheritance diagram for SBMLException:



10.32.1 Detailed Description

Definition at line 13 of file sbml_import.py.

10.33 SbmlImporter Class Reference

The SbmlImporter class generates AMICI C++ files for a model provided in the Systems Biology Markup Language (SBML).

Public Member Functions

- def __init__ (self, SBMLFile, show_sbml_warnings=False)

  Create a new Model instance.
- def reset_symbols (self)

  Reset the symbols attribute to default values.
- def loadSBMLFile (self, SBMLFile)

  Parse the provided SBML file.
- def sbml2amici (self, modelName, output_dir=None, observables=None, constantParameters=None, sigmas=None, verbose=False, assume_pow_positivity=False, compiler=None, allow_reinit_fixpar_↩initcond=True)

  Generate AMICI C++ files for the model provided to the constructor.
- def processSBML (self, constantParameters=None)

  Read parameters, species, reactions, and so on from SBML model.
- def checkSupport (self)

  Check whether all required SBML features are supported.
- def processSpecies (self)

  Get species information from SBML model.
- def processParameters (self, constantParameters=None)

  Get parameter information from SBML model.
- def processCompartments (self)

  Get compartment information, stoichiometric matrix and fluxes from SBML model.

- def processReactions (self)

  Get reactions from SBML model.
- def processRules (self)

  Process Rules defined in the SBML model.
- def processVolumeConversion (self)

  Convert equations from amount to volume.
- def processTime (self)

  Convert time_symbol into cpp variable.
- def processObservables (self, observables, sigmas)

  Perform symbolic computations required for objective function evaluation.
- def replaceInAllExpressions (self, old, new)

  Replace 'old' by 'new' in all symbolic expressions.
- def cleanReservedSymbols (self)

  Remove all reserved symbols from self.symbols.
- def replaceSpecialConstants (self)

  Replace all special constants by their respective SBML csymbol definition.

Public Attributes

- show_sbml_warnings

  indicates whether libSBML warnings should be
- symbols

  dict carrying symbolic definitions
  ***Type**: dict*
- SBMLreader

  the libSBML sbml reader [!not storing this will result
- sbml_doc

  document carrying the sbml definition [!not storing this
- sbml

  sbml definition [!not storing this will result in a segfault!]
- speciesIndex

  maps species names to indices
  ***Type**: dict*
- speciesCompartment

  compartment for each species
  ***Type**:*
- constantSpecies

  ids of species that are marked as constant
  ***Type**: list*
- boundaryConditionSpecies

  ids of species that are marked as boundary
- speciesHasOnlySubstanceUnits

  flags indicating whether a species has
- speciesConversionFactor

  conversion factors for every species
  ***Type**:*
- compartmentSymbols

  compartment ids
  ***Type**: sympy.Matrix*
- compartmentVolume

numeric/symbolic compartment volumes
Type:

- stoichiometricMatrix

  stoichiometric matrix of the model
  Type:

- fluxVector

  reaction kinetic laws
  Type: *sympy.Matrix*

10.33.1 Detailed Description

Definition at line 35 of file sbml_import.py.

10.33.2 Constructor & Destructor Documentation

10.33.2.1 __init__()

```
def __init__ (
              self,
              SBMLFile,
              show_sbml_warnings = False )
```

Parameters

SBMLFile	Path to SBML file where the model is specified **Type**: string
show_sbml_warnings	indicates whether libSBML warnings should be displayed **Type**: bool

Returns

SbmlImporter instance with attached SBML document

Definition at line 143 of file sbml_import.py.

10.33.3 Member Function Documentation

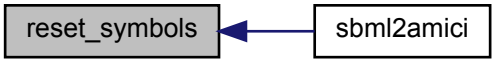
10.33.3.1 reset_symbols()

```
def reset_symbols (
              self )
```

Returns

Definition at line 162 of file sbml_import.py.

Here is the caller graph for this function:



10.33.3.2 loadSBMLFile()

```
def loadSBMLFile (
              self,
              SBMLFile )
```

Parameters

SBMLFile	path to SBML file **Type**: str

Returns

Definition at line 175 of file sbml_import.py.

10.33.3.3 sbml2amici()

```
def sbml2amici (
              self,
              modelName,
              output_dir = None,
              observables = None,
              constantParameters = None,
              sigmas = None,
              verbose = False,
              assume_pow_positivity = False,
              compiler = None,
              allow_reinit_fixpar_initcond = True )
```

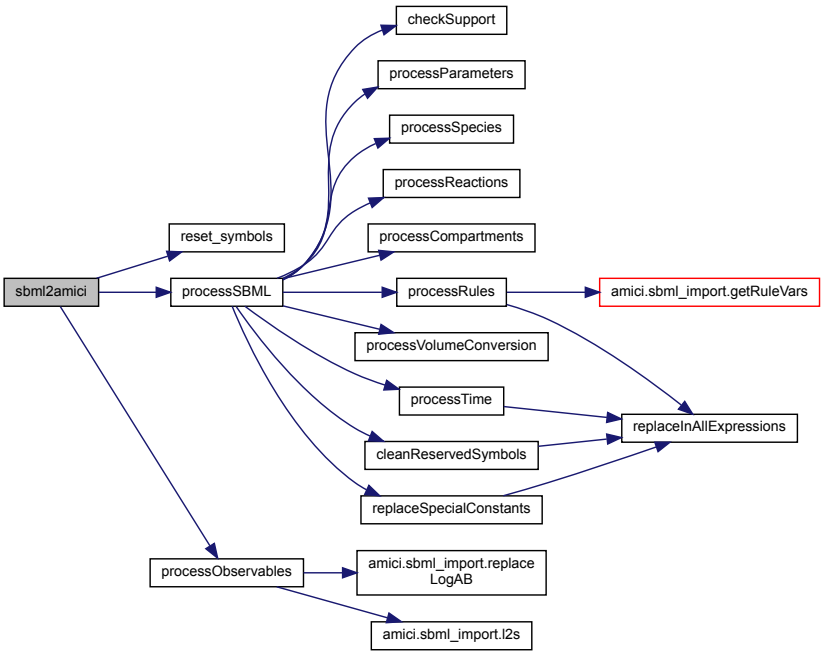
Parameters

modelName	name of the model/model directory **Type**: str
output_dir	see sbml_import.setPaths() **Type**: str
observables	dictionary(observableId:{'name':observableName (optional), 'formula':formulaString)}) to be added to the model **Type**: dict
sigmas	dictionary(observableId: sigma value or (existing) parameter name) **Type**: dict
constantParameters	list of SBML Ids identifying constant parameters **Type**: dict
verbose	more verbose output if True **Type**: bool
assume_pow_positivity	if set to true, a special pow function is used to avoid problems with state variables that may become negative due to numerical errors **Type**: bool
compiler	distutils/setuptools compiler selection to build the python extension **Type**: str
allow_reinit_fixpar_initcond	see ode_export.ODEExporter

Returns

Definition at line 246 of file sbml_import.py.

Here is the call graph for this function:



10.33.3.4 processSBML()

```
def processSBML (
            self,
            constantParameters = None )
```

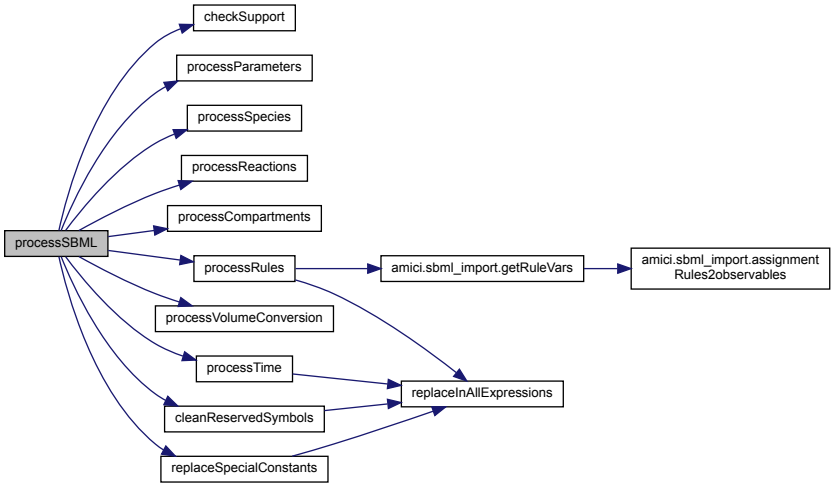
Parameters

constantParameters	SBML Ids identifying constant parameters **Type**: list

Returns

Definition at line 285 of file sbml_import.py.

Here is the call graph for this function:



Here is the caller graph for this function:

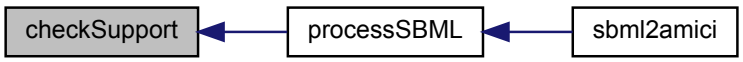
10.33.3.5 checkSupport()

```
def checkSupport (
            self )
```

Returns

Definition at line 310 of file sbml_import.py.

Here is the caller graph for this function:



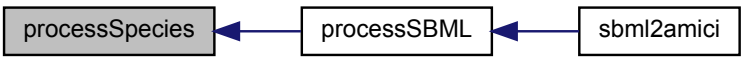
10.33.3.6 processSpecies()

```
def processSpecies (
            self )
```

Returns

Definition at line 347 of file sbml_import.py.

Here is the caller graph for this function:



10.33.3.7 processParameters()

```
def processParameters (
            self,
            constantParameters = None )
```

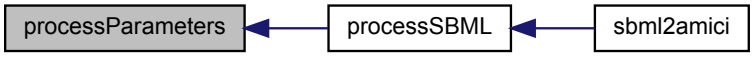
Parameters

constantParameters	SBML Ids identifying constant parameters **Type**: list

Returns

Definition at line 439 of file sbml_import.py.

Here is the caller graph for this function:



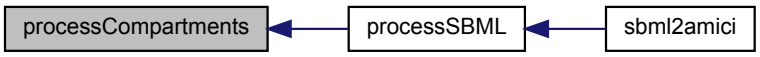
10.33.3.8 processCompartments()

```
def processCompartments (
              self )
```

Returns

Definition at line 516 of file sbml_import.py.

Here is the caller graph for this function:



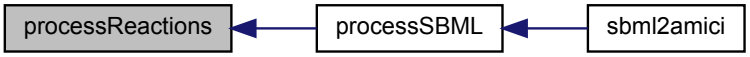
10.33.3.9 processReactions()

```
def processReactions (
              self )
```

Returns

Definition at line 551 of file sbml_import.py.

Here is the caller graph for this function:



10.33.3.10 processRules()

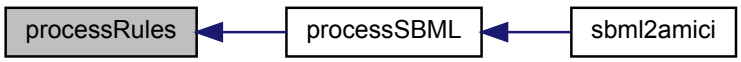
```
def processRules (
              self )
```

Returns

Definition at line 663 of file sbml_import.py.

Here is the call graph for this function:

Here is the caller graph for this function:



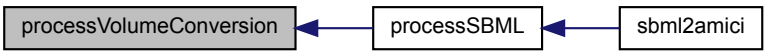
10.33.3.11 processVolumeConversion()

```
def processVolumeConversion (
              self )
```

Returns

Definition at line 740 of file sbml_import.py.

Here is the caller graph for this function:



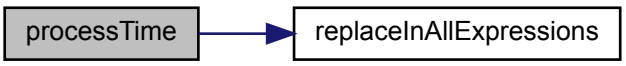
10.33.3.12 processTime()

```
def processTime (
              self )
```

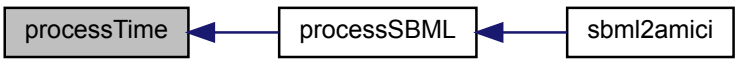
Returns

Definition at line 762 of file sbml_import.py.

Here is the call graph for this function:



Here is the caller graph for this function:



10.33.3.13 processObservables()

```
def processObservables (
              self,
              observables,
              sigmas )
```

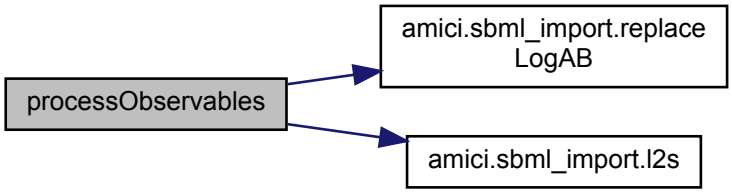
Parameters

observables	dictionary(observableId:{'name':observableName (optional), 'formula':formulaString)}) to be added to the model **Type**: dict
sigmas	dictionary(observableId: sigma value or (existing) parameter name) **Type**: dict

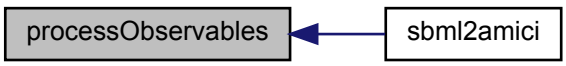
Returns

Definition at line 784 of file sbml_import.py.

Here is the call graph for this function:



Here is the caller graph for this function:



10.33.3.14 replaceInAllExpressions()

```
def replaceInAllExpressions (
              self,
              old,
              new )
```

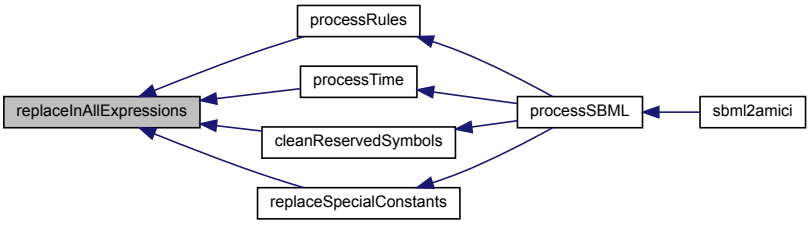
Parameters

old	symbolic variables to be replaced **Type**: symengine.Symbol
new	replacement symbolic variables **Type**: symengine.Symbol

Returns

Definition at line 898 of file sbml_import.py.

Here is the caller graph for this function:



10.33.3.15 cleanReservedSymbols()

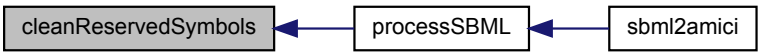
```
def cleanReservedSymbols (
              self )
```

Returns

Definition at line 925 of file sbml_import.py.

Here is the call graph for this function:

Here is the caller graph for this function:



10.33.3.16 replaceSpecialConstants()

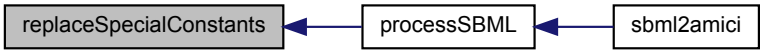
```
def replaceSpecialConstants (
              self )
```

Returns

Definition at line 946 of file sbml_import.py.

Here is the call graph for this function:

Here is the caller graph for this function:

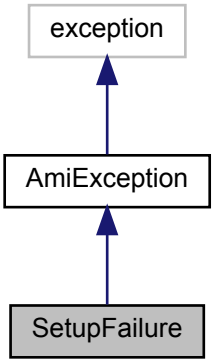


10.34 SetupFailure Class Reference

setup failure exception this exception should be thrown when the solver setup failed for this exception we can assume that we cannot recover from the exception and an error will be thrown

```
#include <exception.h>
```

Inheritance diagram for SetupFailure:



Public Member Functions

- SetupFailure (const char *msg)

10.34.1 Detailed Description

Definition at line 188 of file exception.h.

10.34.2 Constructor & Destructor Documentation

10.34.2.1 SetupFailure()

```
SetupFailure (
            const char * msg )
```

constructor, simply calls AmiException constructor

Parameters

msg	

Definition at line 193 of file exception.h.

10.35 Solver Class Reference

```
#include <solver.h>
```

Public Member Functions

- Solver (const Solver &other)

  Solver copy constructor.
- virtual Solver ∗ clone () const =0

  Clone this instance.
- void setup (AmiVector ∗x, AmiVector ∗dx, AmiVectorArray ∗sx, AmiVectorArray ∗sdx, Model ∗model)

  Initialises the ami memory object and applies specified options.
- void setupAMIB (BackwardProblem ∗bwd, Model ∗model)
- virtual void getSens (realtype ∗tret, AmiVectorArray ∗yySout) const =0
- void getDiagnosis (const int it, ReturnData ∗rdata) const
- void getDiagnosisB (const int it, ReturnData ∗rdata, int which) const
- virtual void getRootInfo (int ∗rootsfound) const =0
- virtual void reInit (realtype t0, AmiVector ∗yy0, AmiVector ∗yp0)=0
- virtual void sensReInit (AmiVectorArray ∗yS0, AmiVectorArray ∗ypS0)=0
- virtual void calcIC (realtype tout1, AmiVector ∗x, AmiVector ∗dx)=0
- virtual void calcICB (int which, realtype tout1, AmiVector ∗xB, AmiVector ∗dxB)=0
- virtual int solve (realtype tout, AmiVector ∗yret, AmiVector ∗ypret, realtype ∗tret, int itask)=0
- virtual int solveF (realtype tout, AmiVector ∗yret, AmiVector ∗ypret, realtype ∗tret, int itask, int ∗ncheckPtr)=0
- virtual void solveB (realtype tBout, int itaskB)=0
- virtual void setStopTime (realtype tstop)=0
- virtual void reInitB (int which, realtype tB0, AmiVector ∗yyB0, AmiVector ∗ypB0)=0
- virtual void getB (int which, realtype ∗tret, AmiVector ∗yy, AmiVector ∗yp) const =0
- virtual void getQuadB (int which, realtype ∗tret, AmiVector ∗qB) const =0
- virtual void quadReInitB (int which, AmiVector ∗yQB0)=0
- virtual void turnOffRootFinding ()=0
- SensitivityMethod getSensitivityMethod () const
- void setSensitivityMethod (SensitivityMethod sensi_meth)

  setSensitivityMethod
- int getNewtonMaxSteps () const

  getNewtonMaxSteps
- void setNewtonMaxSteps (int newton_maxsteps)

  setNewtonMaxSteps
- bool getNewtonPreequilibration () const

  getNewtonPreequilibration
- void setNewtonPreequilibration (bool newton_preeq)

  setNewtonPreequilibration
- int getNewtonMaxLinearSteps () const

  getNewtonMaxLinearSteps
- void setNewtonMaxLinearSteps (int newton_maxlinsteps)

  setNewtonMaxLinearSteps
- SensitivityOrder getSensitivityOrder () const

  returns the sensitvity order
- void setSensitivityOrder (SensitivityOrder sensi)

sets the sensitvity order

- double getRelativeTolerance () const

  returns the relative tolerances for the forward & backward problem
- void setRelativeTolerance (double rtol)

  sets the relative tolerances for the forward & backward problem
- double getAbsoluteTolerance () const

  returns the absolute tolerances for the forward & backward problem
- void setAbsoluteTolerance (double atol)

  sets the absolute tolerances for the forward & backward problem
- double getRelativeToleranceSensi () const

  returns the relative tolerances for the forward sensitivity problem
- void setRelativeToleranceSensi (double rtol)

  sets the relative tolerances for the forward sensitivity problem
- double getAbsoluteToleranceSensi () const

  returns the absolute tolerances for the forward sensitivity problem
- void setAbsoluteToleranceSensi (double atol)

  sets the absolute tolerances for the forward sensitivity problem
- double getRelativeToleranceQuadratures () const

  returns the relative tolerance for the quadrature problem
- void setRelativeToleranceQuadratures (double rtol)

  sets the relative tolerance for the quadrature problem
- double getAbsoluteToleranceQuadratures () const

  returns the absolute tolerance for the quadrature problem
- void setAbsoluteToleranceQuadratures (double atol)

  sets the absolute tolerance for the quadrature problem
- double getRelativeToleranceSteadyState () const

  returns the relative tolerance for the steady state problem
- void setRelativeToleranceSteadyState (double rtol)

  sets the relative tolerance for the steady state problem
- double getAbsoluteToleranceSteadyState () const

  returns the absolute tolerance for the steady state problem
- void setAbsoluteToleranceSteadyState (double atol)

  sets the absolute tolerance for the steady state problem
- double getRelativeToleranceSteadyStateSensi () const

  returns the relative tolerance for the sensitivities of the steady state problem
- void setRelativeToleranceSteadyStateSensi (double rtol)

  sets the relative tolerance for the sensitivities of the steady state problem
- double getAbsoluteToleranceSteadyStateSensi () const

  returns the absolute tolerance for the sensitivities of the steady state problem
- void setAbsoluteToleranceSteadyStateSensi (double atol)

  sets the absolute tolerance for the sensitivities of the steady state problem
- int getMaxSteps () const

  returns the maximum number of solver steps for the forward problem
- void setMaxSteps (int maxsteps)

  sets the maximum number of solver steps for the forward problem
- int getMaxStepsBackwardProblem () const

  returns the maximum number of solver steps for the backward problem
- void setMaxStepsBackwardProblem (int maxsteps)

  sets the maximum number of solver steps for the backward problem
- LinearMultistepMethod getLinearMultistepMethod () const

  returns the linear system multistep method

- void setLinearMultistepMethod (LinearMultistepMethod lmm)

  sets the linear system multistep method
- NonlinearSolverIteration getNonlinearSolverIteration () const

  returns the nonlinear system solution method
- void setNonlinearSolverIteration (NonlinearSolverIteration iter)

  sets the nonlinear system solution method
- InterpolationType getInterpolationType () const

  getInterpolationType
- void setInterpolationType (InterpolationType interpType)

  sets the interpolation of the forward solution that is used for the backwards problem
- StateOrdering getStateOrdering () const

  sets KLU state ordering mode
- void setStateOrdering (StateOrdering ordering)

  sets KLU state ordering mode (only applies when linsol is set to amici.AMICI_KLU)
- booleantype getStabilityLimitFlag () const

  returns stability limit detection mode
- void setStabilityLimitFlag (booleantype stldet)

  set stability limit detection mode
- LinearSolver getLinearSolver () const

  getLinearSolver
- void setLinearSolver (LinearSolver linsol)

  setLinearSolver
- InternalSensitivityMethod getInternalSensitivityMethod () const

  returns the internal sensitivity method
- void setInternalSensitivityMethod (InternalSensitivityMethod ism)

  sets the internal sensitivity method

Protected Member Functions

- virtual void init (AmiVector *x, AmiVector *dx, realtype t)=0
- virtual void binit (int which, AmiVector *xB, AmiVector *dxB, realtype t)=0
- virtual void qbinit (int which, AmiVector *qBdot)=0
- virtual void rootInit (int ne)=0
- virtual void sensInit1 (AmiVectorArray *sx, AmiVectorArray *sdx, int nplist)=0
- virtual void setDenseJacFn ()=0
- virtual void setSparseJacFn ()=0
- virtual void setBandJacFn ()=0
- virtual void setJacTimesVecFn ()=0
- virtual void setDenseJacFnB (int which)=0
- virtual void setSparseJacFnB (int which)=0
- virtual void setBandJacFnB (int which)=0
- virtual void setJacTimesVecFnB (int which)=0
- virtual void allocateSolver ()=0
- virtual void setSStolerances (double rtol, double atol)=0
- virtual void setSensSStolerances (double rtol, double *atol)=0
- virtual void setSensErrCon (bool error_corr)=0
- virtual void setQuadErrConB (int which, bool flag)=0
- virtual void setErrHandlerFn ()=0
- virtual void setUserData (Model *model)=0
- virtual void setUserDataB (int which, Model *model)=0
- virtual void setMaxNumSteps (long int mxsteps)=0
- virtual void setMaxNumStepsB (int which, long int mxstepsB)=0

- virtual void setStabLimDet (int stldet)=0
- virtual void setStabLimDetB (int which, int stldet)=0
- virtual void setId (Model ∗model)=0
- virtual void setSuppressAlg (bool flag)=0
- virtual void setSensParams (realtype ∗p, realtype ∗pbar, int ∗plist)=0
- virtual void getDky (realtype t, int k, AmiVector ∗dky) const =0
- virtual void adjInit ()=0
- virtual void allocateSolverB (int ∗which)=0
- virtual void setSStolerancesB (int which, realtype relTolB, realtype absTolB)=0
- virtual void quadSStolerancesB (int which, realtype reltolQB, realtype abstolQB)=0
- virtual void dense (int nx)=0
- virtual void denseB (int which, int nx)=0
- virtual void band (int nx, int ubw, int lbw)=0
- virtual void bandB (int which, int nx, int ubw, int lbw)=0
- virtual void diag ()=0
- virtual void diagB (int which)=0
- virtual void spgmr (int prectype, int maxl)=0
- virtual void spgmrB (int which, int prectype, int maxl)=0
- virtual void spbcg (int prectype, int maxl)=0
- virtual void spbcgB (int which, int prectype, int maxl)=0
- virtual void sptfqmr (int prectype, int maxl)=0
- virtual void sptfqmrB (int which, int prectype, int maxl)=0
- virtual void klu (int nx, int nnz, int sparsetype)=0
- virtual void kluSetOrdering (int ordering)=0
- virtual void kluSetOrderingB (int which, int ordering)=0
- virtual void kluB (int which, int nx, int nnz, int sparsetype)=0
- virtual void getNumSteps (void ∗ami_mem, long int ∗numsteps) const =0
- virtual void getNumRhsEvals (void ∗ami_mem, long int ∗numrhsevals) const =0
- virtual void getNumErrTestFails (void ∗ami_mem, long int ∗numerrtestfails) const =0
- virtual void getNumNonlinSolvConvFails (void ∗ami_mem, long int ∗numnonlinsolvconvfails) const =0
- virtual void getLastOrder (void ∗ami_mem, int ∗order) const =0
- void initializeLinearSolver (const Model ∗model)
- void initializeLinearSolverB (const Model ∗model, const int which)
- virtual int nplist () const =0
- virtual int nx () const =0
- virtual const Model ∗ getModel () const =0
- virtual bool getMallocDone () const =0
- virtual bool getAdjMallocDone () const =0
- virtual void ∗ getAdjBmem (void ∗ami_mem, int which)=0
- void applyTolerances ()
- void applyTolerancesFSA ()
- void applyTolerancesASA (int which)
- void applyQuadTolerancesASA (int which)
- void applySensitivityTolerances ()

Static Protected Member Functions

- static void wrapErrHandlerFn (int error_code, const char ∗module, const char ∗function, char ∗msg, void ∗eh_data)

Protected Attributes

- std::unique_ptr< void, std::function< void(void *)> > solverMemory
- std::vector< std::unique_ptr< void, std::function< void(void *)> > > solverMemoryB
- bool solverWasCalled = false
- InternalSensitivityMethod ism = InternalSensitivityMethod::simultaneous
- LinearMultistepMethod lmm = LinearMultistepMethod::BDF
- NonlinearSolverIteration iter = NonlinearSolverIteration::newton
- InterpolationType interpType = InterpolationType::hermite
- int maxsteps = 10000

Friends

- template<class Archive >
  void boost::serialization::serialize (Archive &ar, Solver &r, const unsigned int version)

  Serialize Solver (see boost::serialization::serialize)
- bool operator== (const Solver &a, const Solver &b)

  Check equality of data members.

10.35.1 Detailed Description

Solver class. provides a generic interface to CVode and IDA solvers, individual realizations are realized in the CVodeSolver and the IDASolver class.

Definition at line 38 of file solver.h.

10.35.2 Constructor & Destructor Documentation

10.35.2.1 Solver()

```
Solver (
            const Solver & other )
```

Parameters

other	

Definition at line 46 of file solver.h.

10.35.3 Member Function Documentation

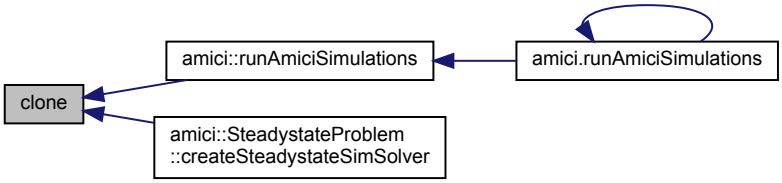
10.35.3.1 clone()

```
virtual Solver* clone ( ) const  [pure virtual]
```

Returns

The clone

Here is the caller graph for this function:



10.35.3.2 setup()

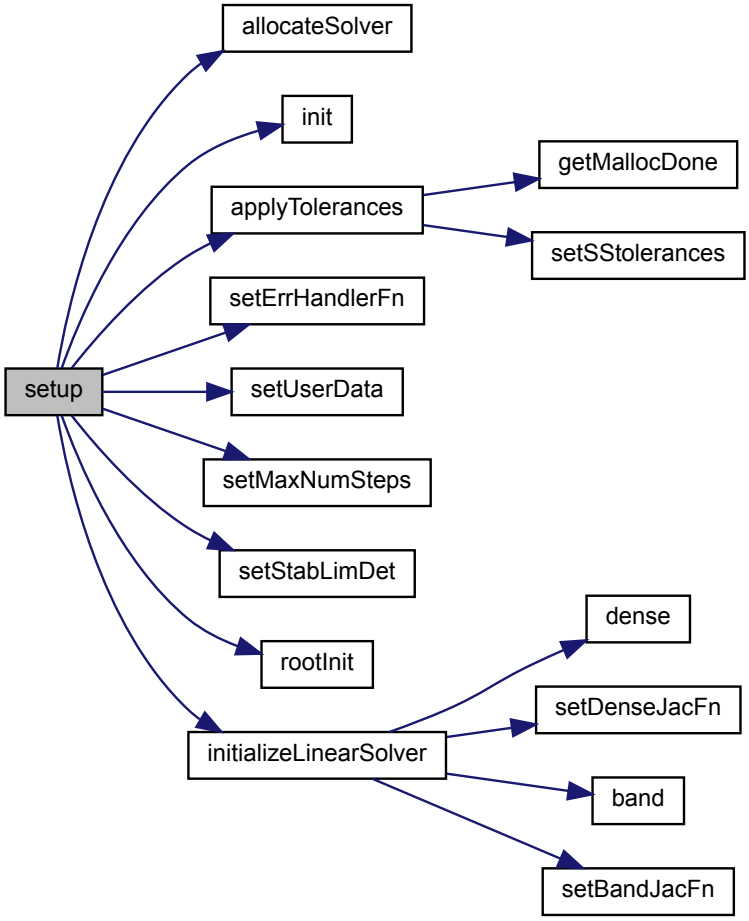
```
void setup (
            AmiVector * x,
            AmiVector * dx,
            AmiVectorArray * sx,
            AmiVectorArray * sdx,
            Model * model )
```

Parameters

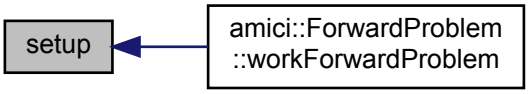
x	state vector
dx	state derivative vector (DAE only)
sx	state sensitivity vector
sdx	state derivative sensitivity vector (DAE only)
model	pointer to the model object

Definition at line 27 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.3 setupAMIB()

```
void setupAMIB (
            BackwardProblem * bwd,
            Model * model )
```

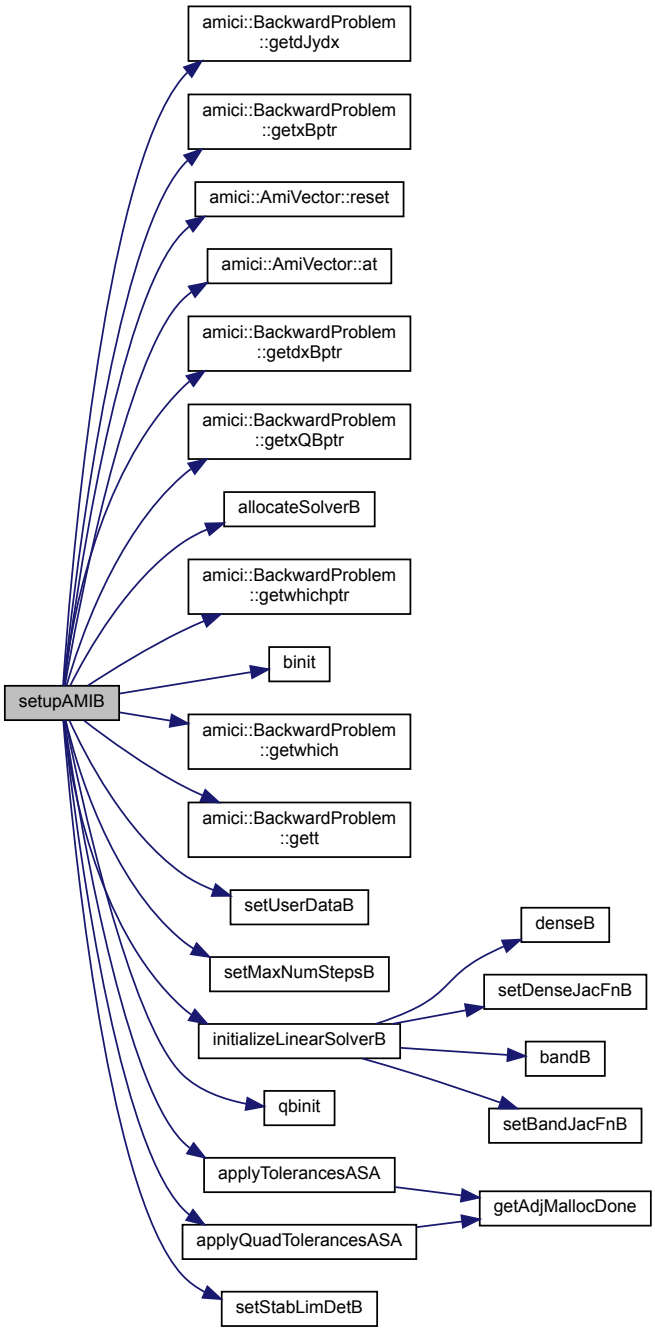
setupAMIB initialises the AMI memory object for the backwards problem

Parameters

bwd	pointer to backward problem
model	pointer to the model object

Definition at line 100 of file solver.cpp.

Here is the call graph for this function:



10.35.3.4 getSens()

```
virtual void getSens (
            realtype * tret,
            AmiVectorArray * yySout ) const  [pure virtual]
```

getSens extracts diagnosis information from solver memory block and writes them into the return data instance

Parameters

tret	time at which the sensitivities should be computed
yySout	vector with sensitivities

10.35.3.5 getDiagnosis()

```
void getDiagnosis (
            const int it,
            ReturnData * rdata ) const
```

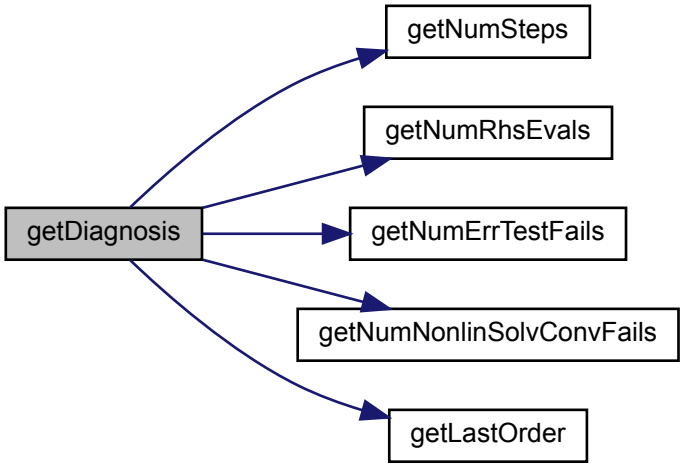
getDiagnosis extracts diagnosis information from solver memory block and writes them into the return data object

Parameters

it	time-point index
rdata	pointer to the return data object

Definition at line 184 of file solver.cpp.

Here is the call graph for this function:



10.35.3.6 getDiagnosisB()

```
void getDiagnosisB (
            const int it,
            ReturnData * rdata,
            int which ) const
```

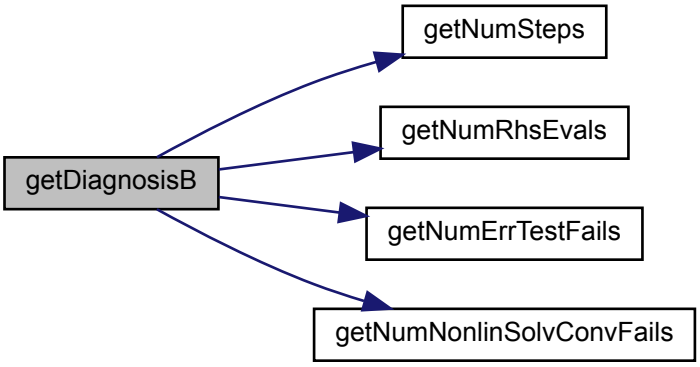
getDiagnosisB extracts diagnosis information from solver memory block and writes them into the return data object for the backward problem

Parameters

it	time-point index
rdata	pointer to the return data object
which	identifier of the backwards problem

Definition at line 204 of file solver.cpp.

Here is the call graph for this function:



10.35.3.7 getRootInfo()

```
virtual void getRootInfo (
            int * rootsfound ) const  [pure virtual]
```

getRootInfo extracts information which event occured

Parameters

rootsfound	array with flags indicating whether the respective event occured

10.35.3.8 reInit()

```
virtual void reInit (
            realtype t0,
            AmiVector * yy0,
            AmiVector * yp0 )  [pure virtual]
```

ReInit reinitializes the states in the solver after an event occurence

Parameters

t0	new timepoint
yy0	new state variables
yp0	new derivative state variables (DAE only)

10.35.3.9 sensReInit()

```
virtual void sensReInit (
            AmiVectorArray * yS0,
            AmiVectorArray * ypS0 )  [pure virtual]
```

SensReInit reinitializes the state sensitivites in the solver after an event occurence

Parameters

yS0	new state sensitivity
ypS0	new derivative state sensitivities (DAE only)

10.35.3.10 calcIC()

```
virtual void calcIC (
            realtype tout1,
            AmiVector * x,
            AmiVector * dx )  [pure virtual]
```

CalcIC calculates consistent initial conditions, assumes initial states to be correct (DAE only)

Parameters

tout1	next timepoint to be computed (sets timescale)
x	initial state variables
dx	initial derivative state variables (DAE only)

10.35.3.11 calcICB()

```
virtual void calcICB (
            int which,
            realtype tout1,
            AmiVector * xB,
            AmiVector * dxB )  [pure virtual]
```

CalcIBC calculates consistent initial conditions for the backwards problem, assumes initial states to be correct (DAE only)

Parameters

which	identifier of the backwards problem
tout1	next timepoint to be computed (sets timescale)
xB	states of final solution of the forward problem
dxB	derivative states of final solution of the forward problem (DAE only)

10.35.3.12 solve()

```
virtual int solve (
            realtype tout,
            AmiVector * yret,
            AmiVector * ypret,
            realtype * tret,
            int itask )  [pure virtual]
```

Solve solves the forward problem until a predefined timepoint

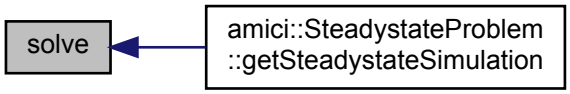
Parameters

tout	timepoint until which simulation should be performed
yret	states
ypret	derivative states (DAE only)
tret	pointer to the time variable
itask	task identifier, can be CV_NORMAL or CV_ONE_STEP

Returns

status flag indicating success of execution

Here is the caller graph for this function:



10.35.3.13 solveF()

```
virtual int solveF (
            realtype tout,
            AmiVector * yret,
            AmiVector * ypret,
            realtype * tret,
            int itask,
            int * ncheckPtr )  [pure virtual]
```

SolveF solves the forward problem until a predefined timepoint (adjoint only)

Parameters

tout	timepoint until which simulation should be performed

Parameters

yret	states
ypret	derivative states (DAE only)
tret	pointer to the time variable
itask	task identifier, can be CV_NORMAL or CV_ONE_STEP
ncheckPtr	pointer to a number that counts the internal checkpoints

Returns

status flag indicating success of execution

10.35.3.14 solveB()

```
virtual void solveB (
            realtype tBout,
            int itaskB )  [pure virtual]
```

SolveB solves the backward problem until a predefined timepoint (adjoint only)

Parameters

tBout	timepoint until which simulation should be performed
itaskB	task identifier, can be CV_NORMAL or CV_ONE_STEP

10.35.3.15 setStopTime()

```
virtual void setStopTime (
            realtype tstop )  [pure virtual]
```

SetStopTime sets a timepoint at which the simulation will be stopped

Parameters

tstop	timepoint until which simulation should be performed

10.35.3.16 reInitB()

```
virtual void reInitB (
            int which,
            realtype tB0,
            AmiVector * yyB0,
            AmiVector * ypB0 )  [pure virtual]
```

ReInitB reinitializes the adjoint states after an event occurence

Parameters

which	identifier of the backwards problem
tB0	new timepoint
yyB0	new adjoint state variables
ypB0	new adjoint derivative state variables (DAE only)

10.35.3.17 getB()

```
virtual void getB (
            int which,
            realtype * tret,
            AmiVector * yy,
            AmiVector * yp ) const  [pure virtual]
```

getB returns the current adjoint states

Parameters

which	identifier of the backwards problem
tret	time at which the adjoint states should be computed
yy	adjoint state variables
yp	adjoint derivative state variables (DAE only)

10.35.3.18 getQuadB()

```
virtual void getQuadB (
            int which,
            realtype * tret,
            AmiVector * qB ) const  [pure virtual]
```

getQuadB returns the current adjoint states

Parameters

which	identifier of the backwards problem
tret	time at which the adjoint states should be computed
qB	adjoint quadrature state variables

10.35.3.19 quadReInitB()

```
virtual void quadReInitB (
            int which,
            AmiVector * yQB0 )  [pure virtual]
```

ReInitB reinitializes the adjoint states after an event occurence

Parameters

which	identifier of the backwards problem
yQB0	new adjoint quadrature state variables

10.35.3.20 turnOffRootFinding()

```
virtual void turnOffRootFinding ( )  [pure virtual]
```

turnOffRootFinding disables rootfinding

10.35.3.21 getSensitivityMethod()

```
SensitivityMethod getSensitivityMethod ( ) const
```

sensitivity method

Returns

method enum

Definition at line 471 of file solver.cpp.

10.35.3.22 setSensitivityMethod()

```
void setSensitivityMethod (
            SensitivityMethod sensi_meth )
```

Parameters

sensi_meth	

Definition at line 475 of file solver.cpp.

Here is the caller graph for this function:

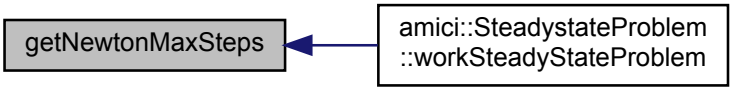
10.35.3.23 getNewtonMaxSteps()

```
int getNewtonMaxSteps ( ) const
```

Returns

Definition at line 479 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.24 setNewtonMaxSteps()

```
void setNewtonMaxSteps (
            int newton_maxsteps )
```

Parameters

newton_maxsteps	

Definition at line 483 of file solver.cpp.

Here is the caller graph for this function:

10.35.3.25 getNewtonPreequilibration()

```
bool getNewtonPreequilibration ( ) const
```

Returns

Definition at line 489 of file solver.cpp.

10.35.3.26 setNewtonPreequilibration()

```
void setNewtonPreequilibration (
            bool newton_preeq )
```

Parameters

newton_preeq	

Definition at line 493 of file solver.cpp.

Here is the caller graph for this function:

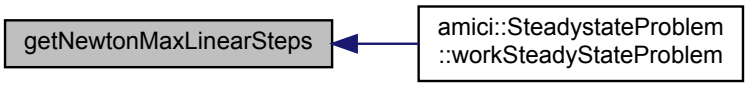
10.35.3.27 getNewtonMaxLinearSteps()

```
int getNewtonMaxLinearSteps ( ) const
```

Returns

Definition at line 497 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.28 setNewtonMaxLinearSteps()

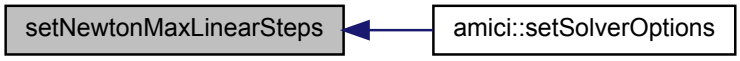
```
void setNewtonMaxLinearSteps (
            int newton_maxlinsteps )
```

Parameters

newton_maxlinsteps	

Definition at line 501 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.29 getSensitivityOrder()

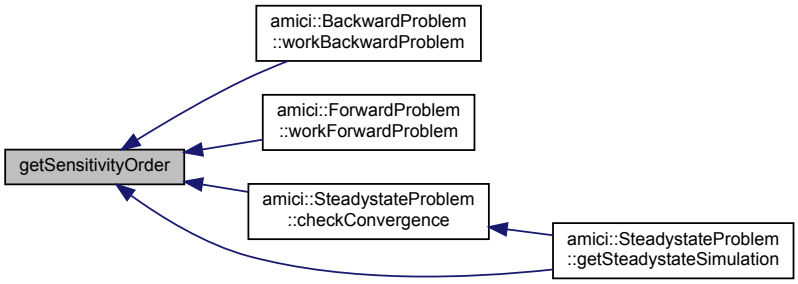
```
SensitivityOrder getSensitivityOrder ( ) const
```

Returns

sensitivity order

Definition at line 507 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.30 setSensitivityOrder()

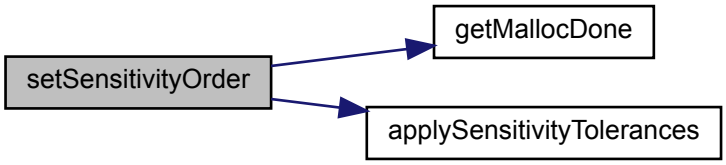
```
void setSensitivityOrder (
            SensitivityOrder sensi )
```

Parameters

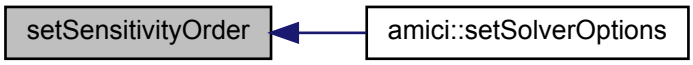
sensi	sensitivity order

Definition at line 511 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.31 getRelativeTolerance()

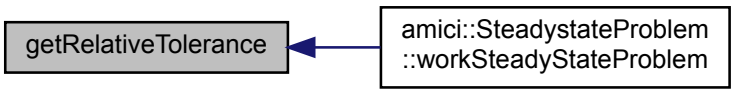
```
double getRelativeTolerance ( ) const
```

Returns

relative tolerances

Definition at line 518 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.32 setRelativeTolerance()

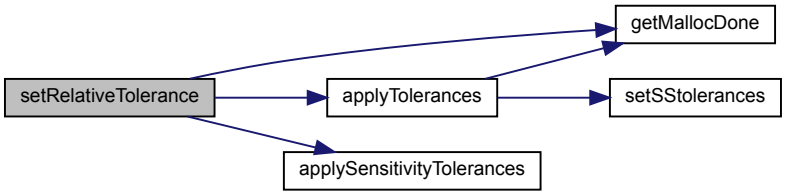
```
void setRelativeTolerance (
            double rtol )
```

Parameters

rtol	relative tolerance (non-negative number)

Definition at line 522 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.35.3.33 getAbsoluteTolerance()

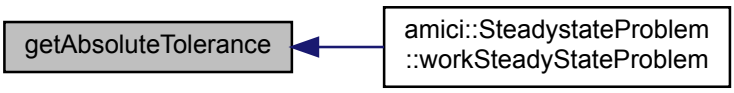
```
double getAbsoluteTolerance ( ) const
```

Returns

absolute tolerances

Definition at line 534 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.34 setAbsoluteTolerance()

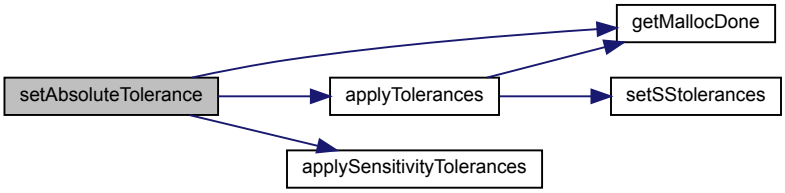
```
void setAbsoluteTolerance (
            double atol )
```

Parameters

atol	absolute tolerance (non-negative number)

Definition at line 538 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.35.3.35 getRelativeToleranceSensi()

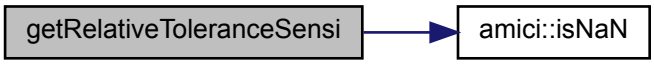
```
double getRelativeToleranceSensi ( ) const
```

Returns

relative tolerances

Definition at line 550 of file solver.cpp.

Here is the call graph for this function:



10.35.3.36 setRelativeToleranceSensi()

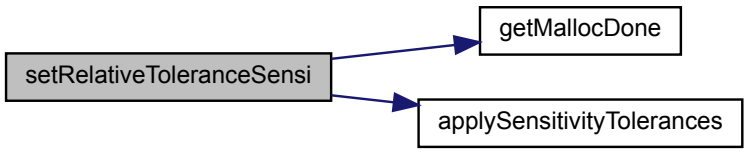
```
void setRelativeToleranceSensi (
            double rtol )
```

Parameters

rtol	relative tolerance (non-negative number)

Definition at line 554 of file solver.cpp.

Here is the call graph for this function:



10.35.3.37 getAbsoluteToleranceSensi()

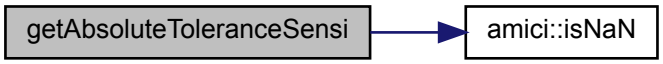
```
double getAbsoluteToleranceSensi ( ) const
```

Returns

absolute tolerances

Definition at line 565 of file solver.cpp.

Here is the call graph for this function:



10.35.3.38 setAbsoluteToleranceSensi()

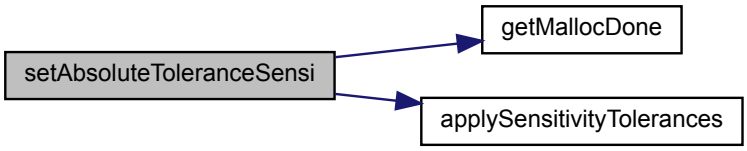
```
void setAbsoluteToleranceSensi (
            double atol )
```

Parameters

atol	absolute tolerance (non-negative number)

Definition at line 569 of file solver.cpp.

Here is the call graph for this function:



10.35.3.39 getRelativeToleranceQuadratures()

```
double getRelativeToleranceQuadratures ( ) const
```

Returns

relative tolerance

Definition at line 580 of file solver.cpp.

10.35.3.40 setRelativeToleranceQuadratures()

```
void setRelativeToleranceQuadratures (
            double rtol )
```

Parameters

rtol	relative tolerance (non-negative number)

Definition at line 584 of file solver.cpp.

Here is the caller graph for this function:

10.35.3.41 getAbsoluteToleranceQuadratures()

```
double getAbsoluteToleranceQuadratures ( ) const
```

Returns

absolute tolerance

Definition at line 598 of file solver.cpp.

10.35.3.42 setAbsoluteToleranceQuadratures()

```
void setAbsoluteToleranceQuadratures (
            double atol )
```

Parameters

atol	absolute tolerance (non-negative number)

Definition at line 602 of file solver.cpp.

Here is the caller graph for this function:

10.35.3.43 getRelativeToleranceSteadyState()

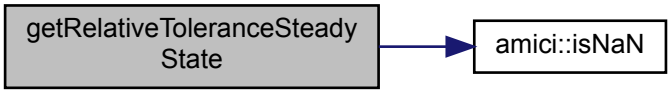
```
double getRelativeToleranceSteadyState ( ) const
```

Returns

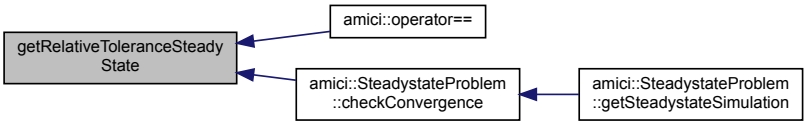
relative tolerance

Definition at line 616 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.44 setRelativeToleranceSteadyState()

```
void setRelativeToleranceSteadyState (
            double rtol )
```

Parameters

rtol	relative tolerance (non-negative number)

Definition at line 620 of file solver.cpp.

10.35.3.45 getAbsoluteToleranceSteadyState()

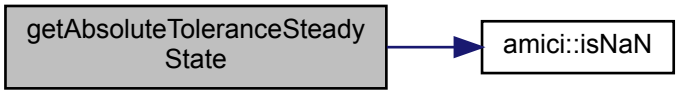
```
double getAbsoluteToleranceSteadyState ( ) const
```

Returns

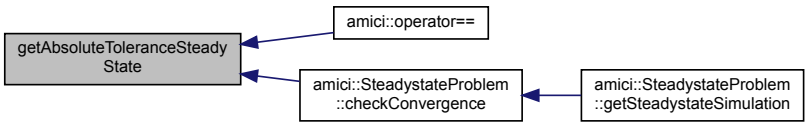
absolute tolerance

Definition at line 627 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.46 setAbsoluteToleranceSteadyState()

```
void setAbsoluteToleranceSteadyState (
            double atol )
```

Parameters

atol	absolute tolerance (non-negative number)

Definition at line 631 of file solver.cpp.

10.35.3.47 getRelativeToleranceSteadyStateSensi()

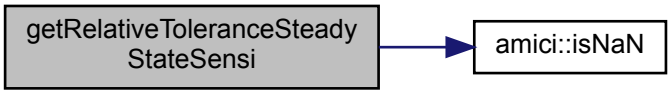
```
double getRelativeToleranceSteadyStateSensi ( ) const
```

Returns

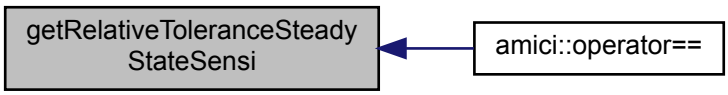
relative tolerance

Definition at line 638 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.48 setRelativeToleranceSteadyStateSensi()

```
void setRelativeToleranceSteadyStateSensi (
            double rtol )
```

Parameters

rtol	relative tolerance (non-negative number)

Definition at line 642 of file solver.cpp.

10.35.3.49 getAbsoluteToleranceSteadyStateSensi()

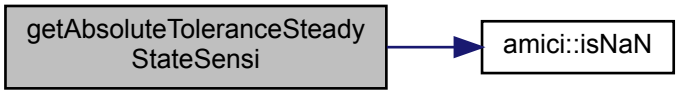
```
double getAbsoluteToleranceSteadyStateSensi ( ) const
```

Returns

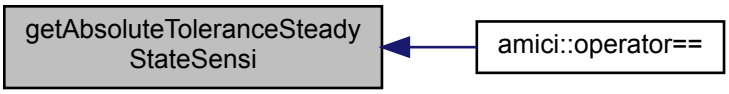
absolute tolerance

Definition at line 649 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.50 setAbsoluteToleranceSteadyStateSensi()

```
void setAbsoluteToleranceSteadyStateSensi (
            double atol )
```

Parameters

atol	absolute tolerance (non-negative number)

Definition at line 653 of file solver.cpp.

10.35.3.51 getMaxSteps()

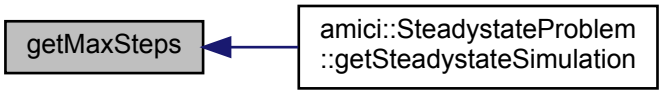
```
int getMaxSteps ( ) const
```

Returns

maximum number of solver steps

Definition at line 660 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.52 setMaxSteps()

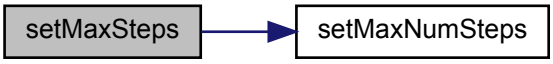
```
void setMaxSteps (
            int maxsteps )
```

Parameters

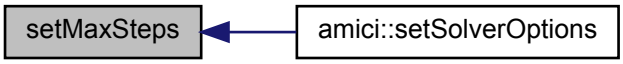
maxsteps	maximum number of solver steps (non-negative number)

Definition at line 664 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.53 getMaxStepsBackwardProblem()

```
int getMaxStepsBackwardProblem ( ) const
```

Returns

maximum number of solver steps

Definition at line 673 of file solver.cpp.

10.35.3.54 setMaxStepsBackwardProblem()

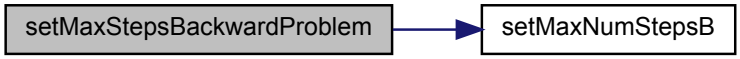
```
void setMaxStepsBackwardProblem (
            int maxsteps )
```

Parameters

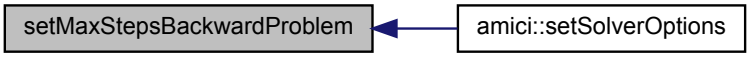
maxsteps	maximum number of solver steps (non-negative number)

Definition at line 677 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.55 getLinearMultistepMethod()

```
LinearMultistepMethod getLinearMultistepMethod ( ) const
```

Returns

linear system multistep method

Definition at line 687 of file solver.cpp.

10.35.3.56 setLinearMultistepMethod()

```
void setLinearMultistepMethod (
            LinearMultistepMethod lmm )
```

Parameters

lmm	linear system multistep method

Definition at line 691 of file solver.cpp.

Here is the caller graph for this function:

10.35.3.57 getNonlinearSolverIteration()

```
NonlinearSolverIteration getNonlinearSolverIteration ( ) const
```

Returns

Definition at line 697 of file solver.cpp.

10.35.3.58 setNonlinearSolverIteration()

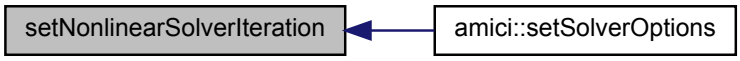
```
void setNonlinearSolverIteration (
            NonlinearSolverIteration iter )
```

Parameters

iter	nonlinear system solution method

Definition at line 701 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.59 getInterpolationType()

```
InterpolationType getInterpolationType ( ) const
```

Returns

Definition at line 707 of file solver.cpp.

10.35.3.60 setInterpolationType()

```
void setInterpolationType (
            InterpolationType interpType )
```

Parameters

interpType	interpolation type

Definition at line 711 of file solver.cpp.

Here is the caller graph for this function:

10.35.3.61 getStateOrdering()

```
StateOrdering getStateOrdering ( ) const
```

Returns

Definition at line 717 of file solver.cpp.

10.35.3.62 setStateOrdering()

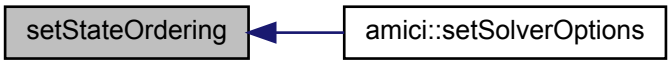
```
void setStateOrdering (
            StateOrdering ordering )
```

Parameters

ordering	state ordering

Definition at line 721 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.63 getStabilityLimitFlag()

```
int getStabilityLimitFlag ( ) const
```

Returns

stldet can be amici.FALSE (deactivated) or amici.TRUE (activated)

Definition at line 731 of file solver.cpp.

10.35.3.64 setStabilityLimitFlag()

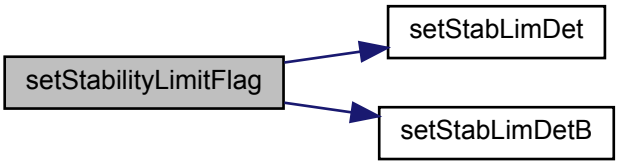
```
void setStabilityLimitFlag (
            booleantype stldet )
```

Parameters

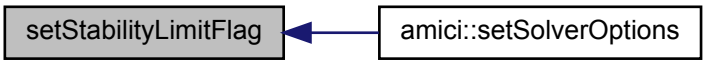
stldet	can be amici.FALSE (deactivated) or amici.TRUE (activated)

Definition at line 735 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



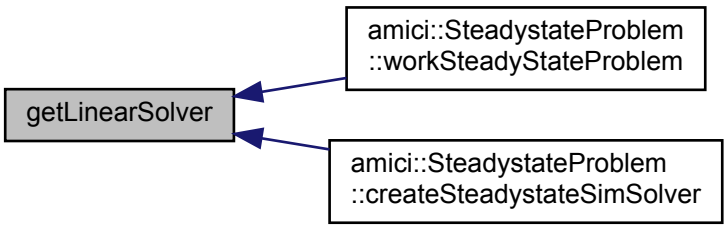
10.35.3.65 getLinearSolver()

```
LinearSolver getLinearSolver ( ) const
```

Returns

Definition at line 748 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.66 setLinearSolver()

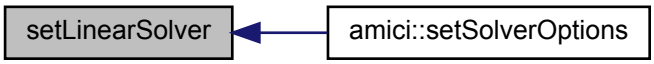
```
void setLinearSolver (
            LinearSolver linsol )
```

Parameters

linsol	

Definition at line 752 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.67 getInternalSensitivityMethod()

```
InternalSensitivityMethod getInternalSensitivityMethod ( ) const
```

Returns

internal sensitivity method

Definition at line 760 of file solver.cpp.

10.35.3.68 setInternalSensitivityMethod()

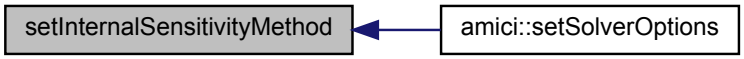
```
void setInternalSensitivityMethod (
            InternalSensitivityMethod ism )
```

Parameters

ism	internal sensitivity method

Definition at line 764 of file solver.cpp.

Here is the caller graph for this function:



10.35.3.69 init()

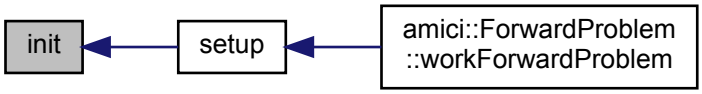
```
virtual void init (
            AmiVector * x,
            AmiVector * dx,
            realtype t )  [protected], [pure virtual]
```

init initialises the states at the specified initial timepoint

Parameters

x	initial state variables
dx	initial derivative state variables (DAE only)
t	initial timepoint

Here is the caller graph for this function:



10.35.3.70 binit()

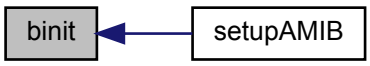
```
virtual void binit (
            int which,
            AmiVector * xB,
            AmiVector * dxB,
            realtype t )  [protected], [pure virtual]
```

binit initialises the adjoint states at the specified final timepoint

Parameters

which	identifier of the backwards problem
xB	initial adjoint state variables
dxB	initial adjoint derivative state variables (DAE only)
t	final timepoint

Here is the caller graph for this function:



10.35.3.71 qbinit()

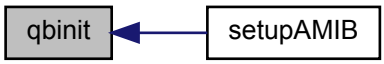
```
virtual void qbinit (
            int which,
            AmiVector * qBdot )  [protected], [pure virtual]
```

qbinit initialises the quadrature states at the specified final timepoint

Parameters

which	identifier of the backwards problem
qBdot	initial adjoint quadrature state variables

Here is the caller graph for this function:



10.35.3.72 rootInit()

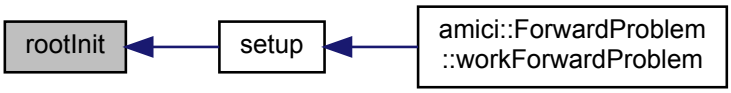
```
virtual void rootInit (
            int ne )  [protected], [pure virtual]
```

RootInit initialises the rootfinding for events

Parameters

ne	number of different events

Here is the caller graph for this function:



10.35.3.73 sensInit1()

```
virtual void sensInit1 (
            AmiVectorArray * sx,
            AmiVectorArray * sdx,
            int nplist )  [protected], [pure virtual]
```

SensInit1 initialises the sensitivities at the specified initial timepoint

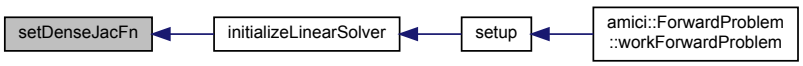
Parameters

sx	initial state sensitivities
sdx	initial derivative state sensitivities (DAE only)
nplist	number parameter wrt which sensitivities are to be computed

10.35.3.74 setDenseJacFn()

```
virtual void setDenseJacFn ( )  [protected], [pure virtual]
```

SetDenseJacFn sets the dense Jacobian function Here is the caller graph for this function:



10.35.3.75 setSparseJacFn()

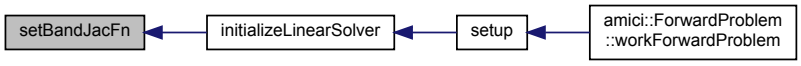
```
virtual void setSparseJacFn ( )  [protected], [pure virtual]
```

SetSparseJacFn sets the sparse Jacobian function

10.35.3.76 setBandJacFn()

```
virtual void setBandJacFn ( )  [protected], [pure virtual]
```

SetBandJacFn sets the banded Jacobian function Here is the caller graph for this function:



10.35.3.77 setJacTimesVecFn()

```
virtual void setJacTimesVecFn ( )  [protected], [pure virtual]
```

SetJacTimesVecFn sets the Jacobian vector multiplication function

10.35.3.78 setDenseJacFnB()

```
virtual void setDenseJacFnB (
            int which )  [protected], [pure virtual]
```

SetDenseJacFn sets the dense Jacobian function

Parameters

which	identifier of the backwards problem

Here is the caller graph for this function:

10.35.3.79 setSparseJacFnB()

```
virtual void setSparseJacFnB (
            int which )  [protected], [pure virtual]
```

SetSparseJacFn sets the sparse Jacobian function

Parameters

which	identifier of the backwards problem

10.35.3.80 setBandJacFnB()

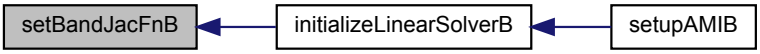
```
virtual void setBandJacFnB (
            int which )  [protected], [pure virtual]
```

SetBandJacFn sets the banded Jacobian function

Parameters

which	identifier of the backwards problem

Here is the caller graph for this function:



10.35.3.81 setJacTimesVecFnB()

```
virtual void setJacTimesVecFnB (
            int which )  [protected], [pure virtual]
```

SetJacTimesVecFn sets the Jacobian vector multiplication function

Parameters

which	identifier of the backwards problem

10.35.3.82 wrapErrHandlerFn()

```
void wrapErrHandlerFn (
            int error_code,
            const char * module,
            const char * function,
            char * msg,
            void * eh_data )  [static], [protected]
```

ErrHandlerFn extracts diagnosis information from solver memory block and writes them into the return data object for the backward problem

Parameters

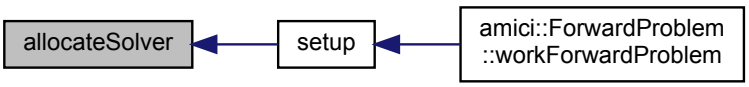
error_code	error identifier
module	name of the module in which the error occured
function	name of the function in which the error occured **Type**: char
msg	error message
eh_data	unused input

Definition at line 149 of file solver.cpp.

10.35.3.83 allocateSolver()

```
virtual void allocateSolver ( )  [protected], [pure virtual]
```

Create specifies solver method and initializes solver memory for the forward problem Here is the caller graph for this function:



10.35.3.84 setSStolerances()

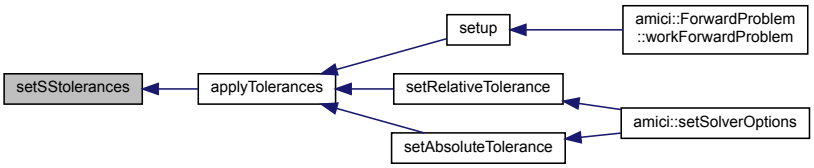
```
virtual void setSStolerances (
            double rtol,
            double atol )  [protected], [pure virtual]
```

SStolerances sets scalar relative and absolute tolerances for the forward problem

Parameters

rtol	relative tolerances
atol	absolute tolerances

Here is the caller graph for this function:



10.35.3.85 setSensSStolerances()

```
virtual void setSensSStolerances (
            double rtol,
            double * atol )  [protected], [pure virtual]
```

SensSStolerances activates sets scalar relative and absolute tolerances for the sensitivity variables

Parameters

rtol	relative tolerances
atol	array of absolute tolerances for every sensitivy variable

10.35.3.86 setSensErrCon()

```
virtual void setSensErrCon (
            bool error_corr )  [protected], [pure virtual]
```

SetSensErrCon specifies whether error control is also enforced for sensitivities for the forward problem

Parameters

error_corr	activation flag

10.35.3.87 setQuadErrConB()

```
virtual void setQuadErrConB (
```

```
int which,
bool flag )  [protected], [pure virtual]
```

SetSensErrCon specifies whether error control is also enforced for the backward quadrature problem

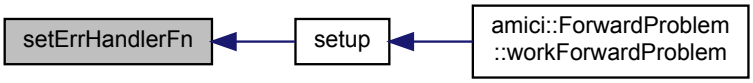
Parameters

which	identifier of the backwards problem
flag	activation flag

10.35.3.88 setErrHandlerFn()

```
virtual void setErrHandlerFn ( )  [protected], [pure virtual]
```

SetErrHandlerFn attaches the error handler function (errMsgIdAndTxt) to the solver Here is the caller graph for this function:



10.35.3.89 setUserData()

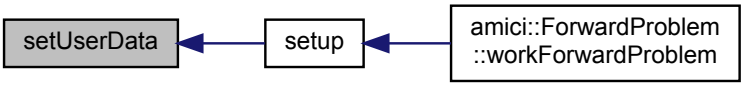
```
virtual void setUserData (
            Model * model )  [protected], [pure virtual]
```

SetUserData attaches the user data instance (here this is a Model) to the forward problem

Parameters

model	Model instance,

Here is the caller graph for this function:



10.35.3.90 setUserDataB()

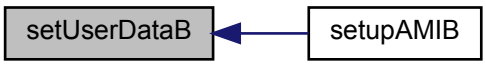
```
virtual void setUserDataB (
            int which,
            Model * model )  [protected], [pure virtual]
```

SetUserDataB attaches the user data instance (here this is a Model) to the backward problem

Parameters

which	identifier of the backwards problem
model	Model instance,

Here is the caller graph for this function:



10.35.3.91 setMaxNumSteps()

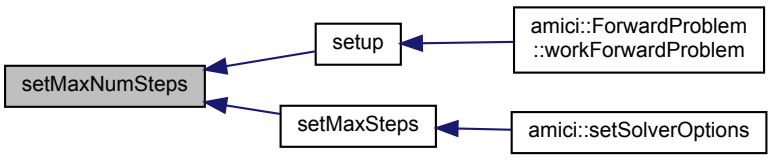
```
virtual void setMaxNumSteps (
            long int mxsteps )  [protected], [pure virtual]
```

SetMaxNumSteps specifies the maximum number of steps for the forward problem

Parameters

mxsteps	number of steps

Here is the caller graph for this function:



10.35.3.92 setMaxNumStepsB()

```
virtual void setMaxNumStepsB (
            int which,
            long int mxstepsB )  [protected], [pure virtual]
```

SetMaxNumStepsB specifies the maximum number of steps for the forward problem

Parameters

which	identifier of the backwards problem
mxstepsB	number of steps

Here is the caller graph for this function:

10.35.3.93 setStabLimDet()

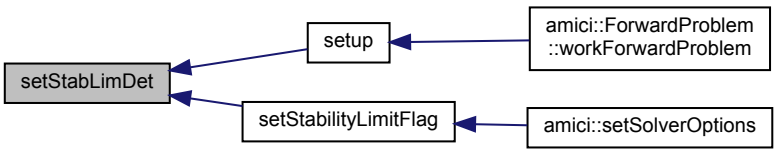
```
virtual void setStabLimDet (
            int stldet )  [protected], [pure virtual]
```

SetStabLimDet activates stability limit detection for the forward problem

Parameters

stldet	flag for stability limit detection (TRUE or FALSE)

Here is the caller graph for this function:



10.35.3.94 setStabLimDetB()

```
virtual void setStabLimDetB (
            int which,
            int stldet )  [protected], [pure virtual]
```

SetStabLimDetB activates stability limit detection for the backward problem

Parameters

which	identifier of the backwards problem
stldet	flag for stability limit detection (TRUE or FALSE)

Here is the caller graph for this function:

10.35.3.95 setId()

```
virtual void setId (
            Model * model )  [protected], [pure virtual]
```

SetId specify algebraic/differential components (DAE only)

Parameters

model	model specification

10.35.3.96 setSuppressAlg()

```
virtual void setSuppressAlg (
            bool flag )  [protected], [pure virtual]
```

SetId deactivates error control for algebraic components (DAE only)

Parameters

flag	deactivation flag

10.35.3.97 setSensParams()

```
virtual void setSensParams (
            realtype * p,
            realtype * pbar,
            int * plist )  [protected], [pure virtual]
```

SetSensParams specifies the scaling and indexes for sensitivity computation

Parameters

p	paramaters
pbar	parameter scaling constants
plist	parameter index list

10.35.3.98 getDky()

```
virtual void getDky (
            realtype t,
            int k,
            AmiVector * dky ) const  [protected], [pure virtual]
```

getDky interpolates the (derivative of the) solution at the requested timepoint

Parameters

t	timepoint
k	derivative order
dky	interpolated solution

10.35.3.99 adjInit()

```
virtual void adjInit ( )  [protected], [pure virtual]
```

AdjInit initializes the adjoint problem

10.35.3.100 allocateSolverB()

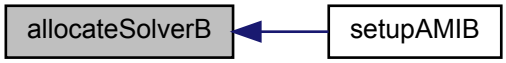
```
virtual void allocateSolverB (
            int * which )  [protected], [pure virtual]
```

specifies solver method and initializes solver memory for the backward problem

Parameters

which	identifier of the backwards problem

Here is the caller graph for this function:



10.35.3.101 setSStolerancesB()

```
virtual void setSStolerancesB (
            int which,
            realtype relTolB,
            realtype absTolB )  [protected], [pure virtual]
```

SStolerancesB sets relative and absolute tolerances for the backward problem

Parameters

which	identifier of the backwards problem
relTolB	relative tolerances
absTolB	absolute tolerances

10.35.3.102 quadSStolerancesB()

```
virtual void quadSStolerancesB (
            int which,
            realtype reltolQB,
            realtype abstolQB )  [protected], [pure virtual]
```

SStolerancesB sets relative and absolute tolerances for the quadrature backward problem

Parameters

which	identifier of the backwards problem
reltolQB	relative tolerances
abstolQB	absolute tolerances

10.35.3.103 dense()

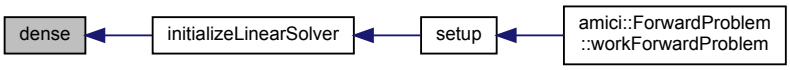
```
virtual void dense (
            int nx )  [protected], [pure virtual]
```

Dense attaches a dense linear solver to the forward problem

Parameters

nx	number of state variables

Here is the caller graph for this function:



10.35.3.104 denseB()

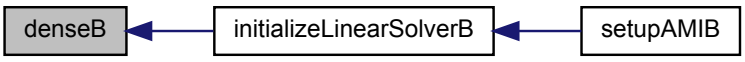
```
virtual void denseB (
            int which,
            int nx )  [protected], [pure virtual]
```

DenseB attaches a dense linear solver to the backward problem

Parameters

which	identifier of the backwards problem
nx	number of state variables

Here is the caller graph for this function:



10.35.3.105 band()

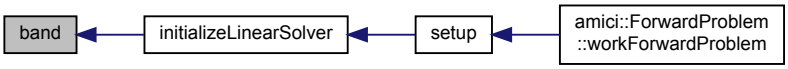
```
virtual void band (
            int nx,
            int ubw,
            int lbw )  [protected], [pure virtual]
```

Band attaches a banded linear solver to the forward problem

Parameters

nx	number of state variables
ubw	upper matrix bandwidth
lbw	lower matrix bandwidth

Here is the caller graph for this function:



10.35.3.106 bandB()

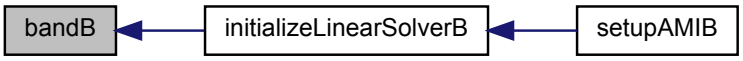
```
virtual void bandB (
            int which,
            int nx,
            int ubw,
            int lbw )  [protected], [pure virtual]
```

BandB attaches a banded linear solver to the backward problem

Parameters

which	identifier of the backwards problem
nx	number of state variables
ubw	upper matrix bandwidth
lbw	lower matrix bandwidth

Here is the caller graph for this function:



10.35.3.107 diag()

```
virtual void diag ( )  [protected], [pure virtual]
```

Diag attaches a diagonal linear solver to the forward problem

10.35.3.108 diagB()

```
virtual void diagB (
            int which )  [protected], [pure virtual]
```

DiagB attaches a diagonal linear solver to the backward problem

Parameters

which	identifier of the backwards problem

10.35.3.109 spgmr()

```
virtual void spgmr (
            int prectype,
            int maxl )  [protected], [pure virtual]
```

DAMISpgmr attaches a scaled predonditioned GMRES linear solver to the forward problem

Parameters

prectype	preconditioner type PREC_NONE, PREC_LEFT, PREC_RIGHT or PREC_BOTH
maxl	maximum Kryloc subspace dimension

10.35.3.110 spgmrB()

```
virtual void spgmrB (
            int which,
```

```
            int prectype,
            int maxl )  [protected], [pure virtual]
```

DAMISpgmrB attaches a scaled predonditioned GMRES linear solver to the backward problem

Parameters

which	identifier of the backwards problem
prectype	preconditioner type PREC_NONE, PREC_LEFT, PREC_RIGHT or PREC_BOTH
maxl	maximum Kryloc subspace dimension

10.35.3.111 spbcg()

```
virtual void spbcg (
            int prectype,
            int maxl )  [protected], [pure virtual]
```

Spbcg attaches a scaled predonditioned Bi-CGStab linear solver to the forward problem

Parameters

prectype	preconditioner type PREC_NONE, PREC_LEFT, PREC_RIGHT or PREC_BOTH
maxl	maximum Kryloc subspace dimension

10.35.3.112 spbcgB()

```
virtual void spbcgB (
            int which,
            int prectype,
            int maxl )  [protected], [pure virtual]
```

SpbcgB attaches a scaled predonditioned Bi-CGStab linear solver to the backward problem

Parameters

which	identifier of the backwards problem
prectype	preconditioner type PREC_NONE, PREC_LEFT, PREC_RIGHT or PREC_BOTH
maxl	maximum Kryloc subspace dimension

10.35.3.113 sptfqmr()

```
virtual void sptfqmr (
            int prectype,
            int maxl )  [protected], [pure virtual]
```

Sptfqmr attaches a scaled predonditioned TFQMR linear solver to the forward problem

Parameters

prectype	preconditioner type PREC_NONE, PREC_LEFT, PREC_RIGHT or PREC_BOTH
maxl	maximum Kryloc subspace dimension

10.35.3.114 sptfqmrB()

```
virtual void sptfqmrB (
            int which,
            int prectype,
            int maxl )  [protected], [pure virtual]
```

SptfqmrB attaches a scaled predonditioned TFQMR linear solver to the backward problem

Parameters

which	identifier of the backwards problem
prectype	preconditioner type PREC_NONE, PREC_LEFT, PREC_RIGHT or PREC_BOTH
maxl	maximum Kryloc subspace dimension

10.35.3.115 klu()

```
virtual void klu (
            int nx,
            int nnz,
            int sparsetype )  [protected], [pure virtual]
```

KLU attaches a sparse linear solver to the forward problem

Parameters

nx	number of state variables
nnz	number of nonzero entries in the jacobian
sparsetype	sparse storage type, CSC_MAT for column matrix, CSR_MAT for row matrix

10.35.3.116 kluSetOrdering()

```
virtual void kluSetOrdering (
            int ordering )  [protected], [pure virtual]
```

KLUSetOrdering sets the ordering for the sparse linear solver of the forward problem

Parameters

ordering	ordering algorithm to reduce fill 0:AMD 1:COLAMD 2: natural ordering

10.35.3.117 kluSetOrderingB()

```
virtual void kluSetOrderingB (
            int which,
            int ordering )  [protected], [pure virtual]
```

KLUSetOrderingB sets the ordering for the sparse linear solver of the backward problem

Parameters

which	identifier of the backwards problem
ordering	ordering algorithm to reduce fill 0:AMD 1:COLAMD 2: natural ordering

10.35.3.118 kluB()

```
virtual void kluB (
            int which,
            int nx,
            int nnz,
            int sparsetype )  [protected], [pure virtual]
```

KLUB attaches a sparse linear solver to the forward problem

Parameters

which	identifier of the backwards problem
nx	number of state variables
nnz	number of nonzero entries in the jacobian
sparsetype	sparse storage type, CSC_MAT for column matrix, CSR_MAT for row matrix

10.35.3.119 getNumSteps()

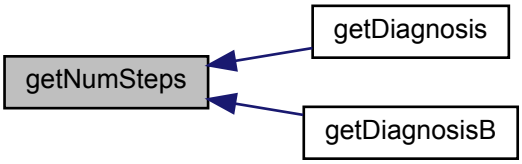
```
virtual void getNumSteps (
            void * ami_mem,
            long int * numsteps ) const  [protected], [pure virtual]
```

getNumSteps reports the number of solver steps

Parameters

ami_mem	pointer to the solver memory instance (can be from forward or backward problem)
numsteps	output array

Here is the caller graph for this function:



10.35.3.120 getNumRhsEvals()

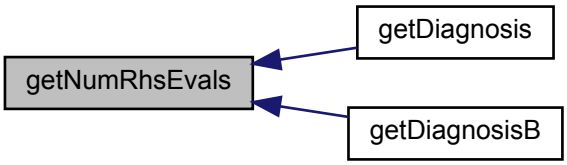
```
virtual void getNumRhsEvals (
            void * ami_mem,
            long int * numrhsevals ) const  [protected], [pure virtual]
```

getNumRhsEvals reports the number of right hand evaluations

Parameters

ami_mem	pointer to the solver memory instance (can be from forward or backward problem)
numrhsevals	output array

Here is the caller graph for this function:



10.35.3.121 getNumErrTestFails()

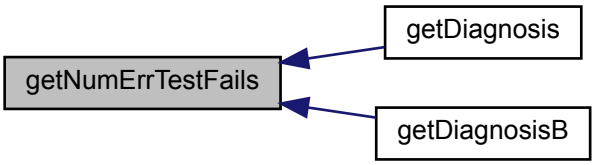
```
virtual void getNumErrTestFails (
            void * ami_mem,
            long int * numerrtestfails ) const  [protected], [pure virtual]
```

getNumErrTestFails reports the number of local error test failures

Parameters

ami_mem	pointer to the solver memory instance (can be from forward or backward problem)
numerrtestfails	output array

Here is the caller graph for this function:



10.35.3.122 getNumNonlinSolvConvFails()

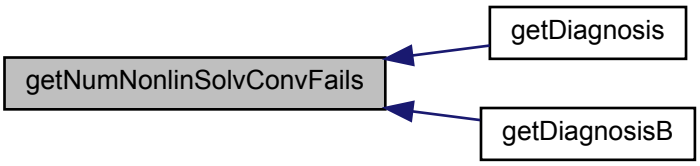
```
virtual void getNumNonlinSolvConvFails (
            void * ami_mem,
            long int * numnonlinsolvconvfails ) const  [protected], [pure virtual]
```

getNumNonlinSolvConvFails reports the number of nonlinear convergence failures

Parameters

ami_mem	pointer to the solver memory instance (can be from forward or backward problem)
numnonlinsolvconvfails	output array

Here is the caller graph for this function:



10.35.3.123 getLastOrder()

```
virtual void getLastOrder (
            void * ami_mem,
            int * order ) const  [protected], [pure virtual]
```

Reports the order of the integration method during the last internal step

Parameters

ami_mem	pointer to the solver memory instance (can be from forward or backward problem)
order	output array

Here is the caller graph for this function:

10.35.3.124 initializeLinearSolver()

```
void initializeLinearSolver (
            const Model * model )  [protected]
```

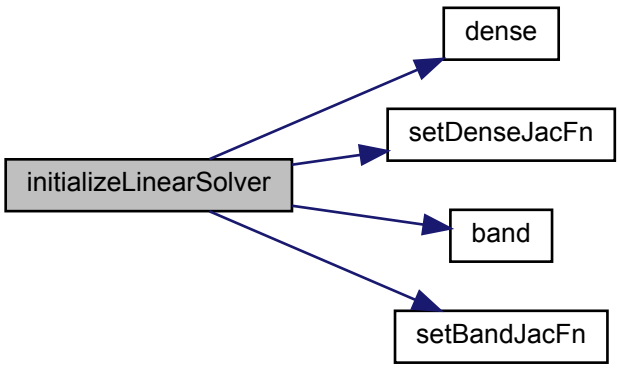
initializeLinearSolver sets the linear solver for the forward problem

Parameters

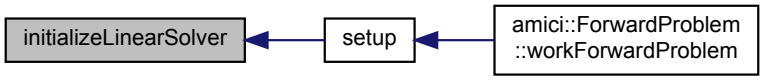
model	pointer to the model object

Definition at line 227 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.125 initializeLinearSolverB()

```
void initializeLinearSolverB (
            const Model * model,
            const int which )  [protected]
```

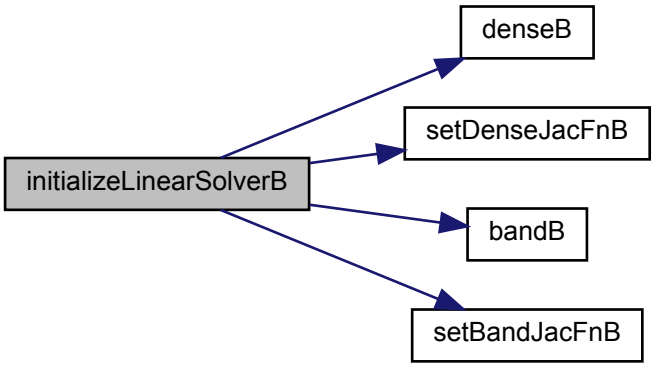
Sets the linear solver for the backward problem

Parameters

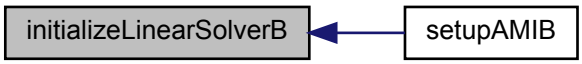
model	pointer to the model object
which	index of the backward problem

Definition at line 304 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.35.3.126 nplist()

```
virtual int nplist ( ) const  [protected], [pure virtual]
```

Accessor function to the number of sensitivity parameters in the model stored in the user data

Returns

number of sensitivity parameters

10.35.3.127 nx()

```
virtual int nx ( ) const  [protected], [pure virtual]
```

Accessor function to the number of state variables in the model stored in the user data

Returns

number of state variables

10.35.3.128 getModel()

```
virtual const Model* getModel ( ) const  [protected], [pure virtual]
```

Accessor function to the model stored in the user data

Returns

user data model

10.35.3.129 getMallocDone()

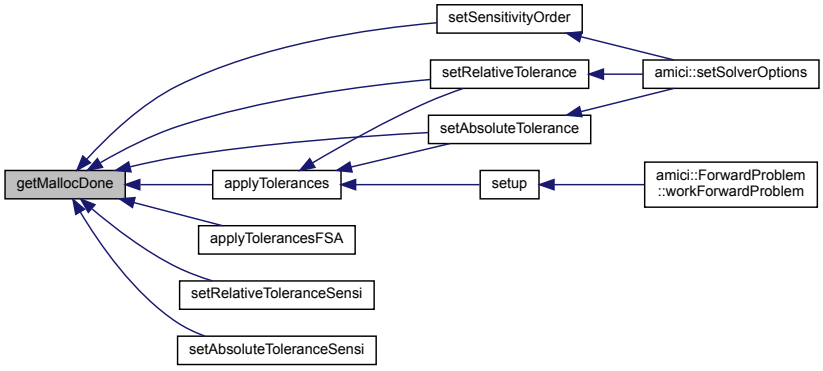
```
virtual bool getMallocDone ( ) const  [protected], [pure virtual]
```

checks whether memory for the forward problem has been allocated

Returns

solverMemory->(cv|ida)__MallocDone

Here is the caller graph for this function:



10.35.3.130 getAdjMallocDone()

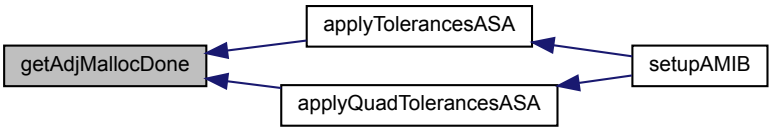
```
virtual bool getAdjMallocDone ( ) const  [protected], [pure virtual]
```

checks whether memory for the backward problem has been allocated

Returns

solverMemory->(cv|ida)__adjMallocDone

Here is the caller graph for this function:



10.35.3.131 getAdjBmem()

```
virtual void* getAdjBmem (
            void * ami_mem,
            int which )  [protected], [pure virtual]
```

getAdjBmem retrieves the solver memory instance for the backward problem

Parameters

which	identifier of the backwards problem
ami_mem	pointer to the forward solver memory instance

Returns

ami_memB pointer to the backward solver memory instance

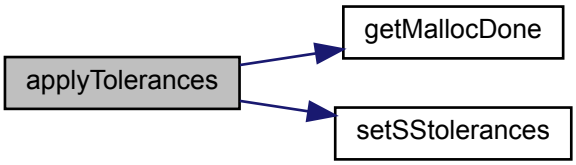
10.35.3.132 applyTolerances()

```
void applyTolerances ( )  [protected]
```

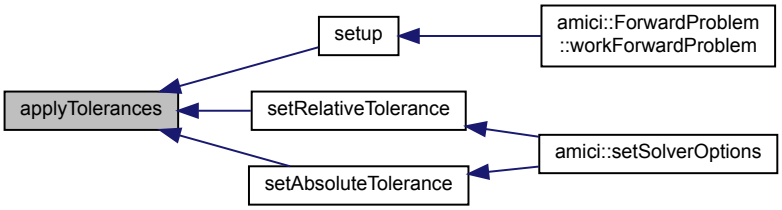
updates solver tolerances according to the currently specified member variables

Definition at line 408 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



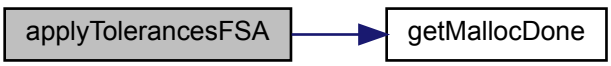
10.35.3.133 applyTolerancesFSA()

```
void applyTolerancesFSA ( ) [protected]
```

updates FSA solver tolerances according to the currently specified member variables

Definition at line 415 of file solver.cpp.

Here is the call graph for this function:



10.35.3.134 applyTolerancesASA()

```
void applyTolerancesASA (
            int which ) [protected]
```

updates ASA solver tolerances according to the currently specified member variables

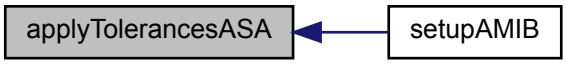
Parameters

which	identifier of the backwards problem

Definition at line 429 of file solver.cpp.

Here is the call graph for this function:

Here is the caller graph for this function:



10.35.3.135 applyQuadTolerancesASA()

```
void applyQuadTolerancesASA (
            int which )  [protected]
```

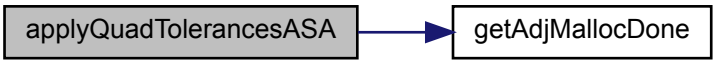
updates ASA quadrature solver tolerances according to the currently specified member variables

Parameters

which	identifier of the backwards problem

Definition at line 440 of file solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

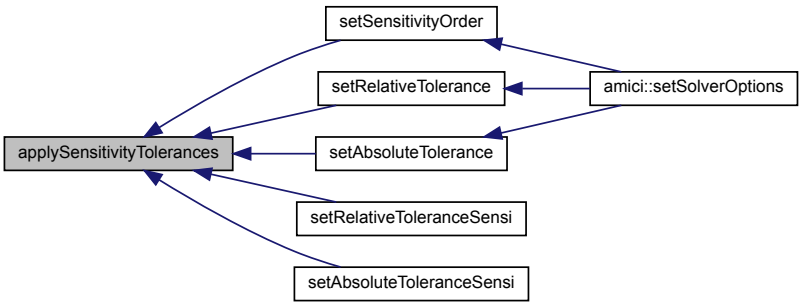
10.35.3.136 applySensitivityTolerances()

```
void applySensitivityTolerances ( ) [protected]
```

updates all senstivivity solver tolerances according to the currently specified member variables

Definition at line 459 of file solver.cpp.

Here is the caller graph for this function:



10.35.4 Friends And Related Function Documentation

10.35.4.1 boost::serialization::serialize

```
void boost::serialization::serialize (
            Archive & ar,
            Solver & r,
            const unsigned int version )  [friend]
```

Parameters

ar	Archive to serialize to
r	Data to serialize
version	Version number

10.35.4.2 operator==

```
bool operator== (
            const Solver & a,
            const Solver & b )  [friend]
```

Parameters

a	
b	

Returns

Definition at line 378 of file solver.cpp.

10.35.5 Member Data Documentation

10.35.5.1 solverMemory

```
std::unique_ptr<void, std::function<void(void *)> > solverMemory  [protected]
```

pointer to solver memory block

Definition at line 1107 of file solver.h.

10.35.5.2 solverMemoryB

```
std::vector<std::unique_ptr<void, std::function<void(void *)> > > solverMemoryB  [protected]
```

pointer to solver memory block

Definition at line 1110 of file solver.h.

10.35.5.3 solverWasCalled

```
bool solverWasCalled = false  [protected]
```

flag indicating whether the solver was called

Definition at line 1113 of file solver.h.

10.35.5.4 ism

```
InternalSensitivityMethod ism = InternalSensitivityMethod::simultaneous  [protected]
```

internal sensitivity method flag used to select the sensitivity solution method. Only applies for Forward Sensitivities.

Definition at line 1117 of file solver.h.

10.35.5.5 lmm

```
LinearMultistepMethod lmm = LinearMultistepMethod::BDF  [protected]
```

specifies the linear multistep method.

Definition at line 1121 of file solver.h.

10.35.5.6 iter

```
NonlinearSolverIteration iter = NonlinearSolverIteration::newton  [protected]
```

specifies the type of nonlinear solver iteration

Definition at line 1126 of file solver.h.

10.35.5.7 interpType

```
InterpolationType interpType = InterpolationType::hermite  [protected]
```

interpolation type for the forward problem solution which is then used for the backwards problem.

Definition at line 1131 of file solver.h.

10.35.5.8 maxsteps

```
int maxsteps = 10000  [protected]
```

maximum number of allowed integration steps

Definition at line 1134 of file solver.h.

10.36 SteadystateProblem Class Reference

The SteadystateProblem class solves a steady-state problem using Newton's method and falls back to integration on failure.

```
#include <steadystateproblem.h>
```

Public Member Functions

- void workSteadyStateProblem (ReturnData ∗rdata, Solver ∗solver, Model ∗model, int it)
- realtype getWrmsNorm (AmiVector const &x, AmiVector const &xdot, realtype atol, realtype rtol)
- bool checkConvergence (const Solver ∗solver, Model ∗model)
- void applyNewtonsMethod (ReturnData ∗rdata, Model ∗model, NewtonSolver ∗newtonSolver, int newton_try)
- void writeNewtonOutput (ReturnData ∗rdata, const Model ∗model, NewtonStatus newton_status, double run_time, int it)
- void getSteadystateSimulation (ReturnData ∗rdata, Solver ∗solver, Model ∗model, int it)
- std::unique_ptr< Solver > createSteadystateSimSolver (Solver ∗solver, Model ∗model, realtype tstart)
- SteadystateProblem (realtype ∗t, AmiVector ∗x, AmiVectorArray ∗sx)

10.36.1 Detailed Description

Definition at line 25 of file steadystateproblem.h.

10.36.2 Constructor & Destructor Documentation

10.36.2.1 SteadystateProblem()

```
SteadystateProblem (
            realtype * t,
            AmiVector * x,
            AmiVectorArray * sx )
```

default constructor

Parameters

t	pointer to time variable
x	pointer to state variables
sx	pointer to state sensitivity variables

Definition at line 108 of file steadystateproblem.h.

10.36.3 Member Function Documentation

10.36.3.1 workSteadyStateProblem()

```
void workSteadyStateProblem (
            ReturnData * rdata,
            Solver * solver,
            Model * model,
            int it )
```

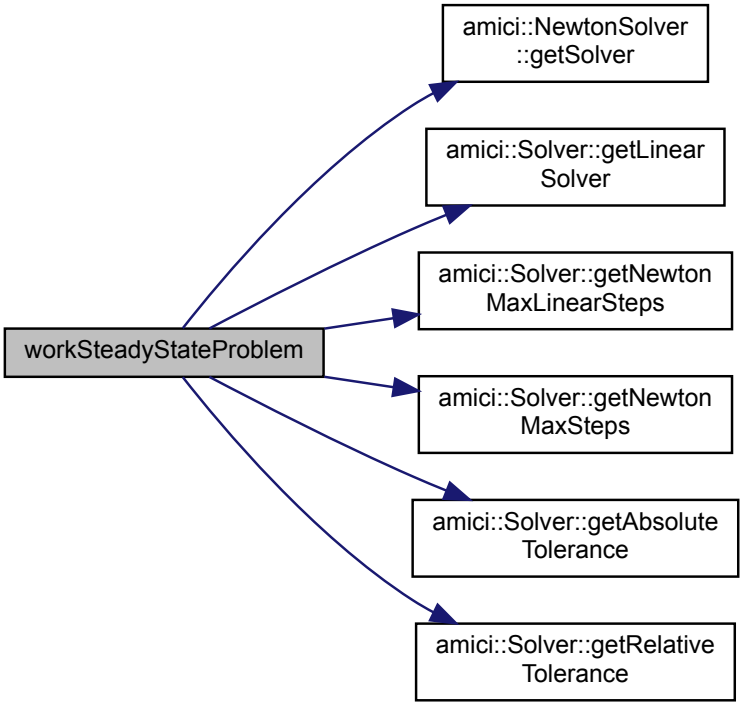
Tries to determine the steady state of the ODE system by a Newton solver, uses forward intergration, if the Newton solver fails, restarts Newton solver, if integration fails. Computes steady state sensitivities

Parameters

solver	pointer to the AMICI solver object
model	pointer to the AMICI model object
it	integer with the index of the current time step
rdata	pointer to the return data object

Definition at line 21 of file steadystateproblem.cpp.

Here is the call graph for this function:



10.36.3.2 getWrmsNorm()

```
realtype getWrmsNorm (
            AmiVector const & x,
            AmiVector const & xdot,
            realtype atol,
            realtype rtol )
```

Computes the weighted root mean square of xdot the weights are computed according to x: w_i = 1 / (rtol ∗ x_i + atol)

Parameters

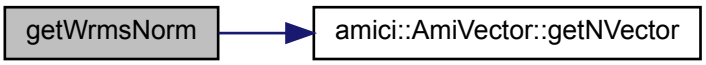
x	current state
xdot	current rhs
atol	absolute tolerance
rtol	relative tolerance

Returns

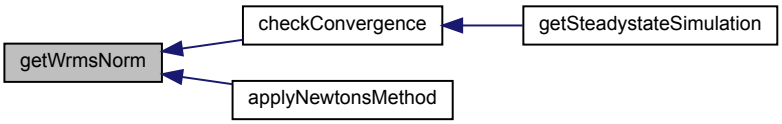
root-mean-square norm

Definition at line 94 of file steadystateproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.36.3.3 checkConvergence()

```
bool checkConvergence (
            const Solver * solver,
            Model * model )
```

Checks convergence for state and respective sensitivities

Parameters

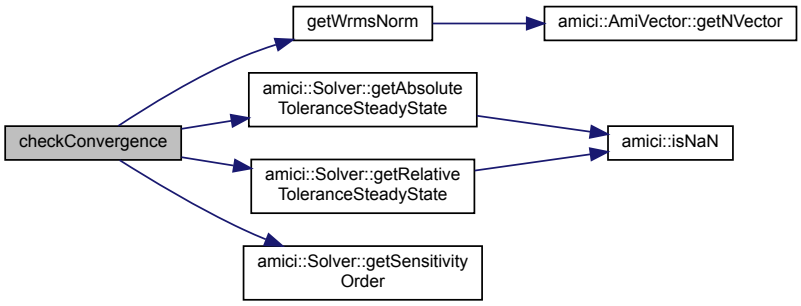
solver	Solver instance
model	instance

Returns

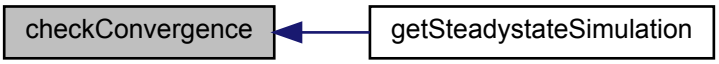
boolean indicating convergence

Definition at line 106 of file steadystateproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.36.3.4 applyNewtonsMethod()

```
void applyNewtonsMethod (
            ReturnData * rdata,
            Model * model,
            NewtonSolver * newtonSolver,
            int newton_try )
```

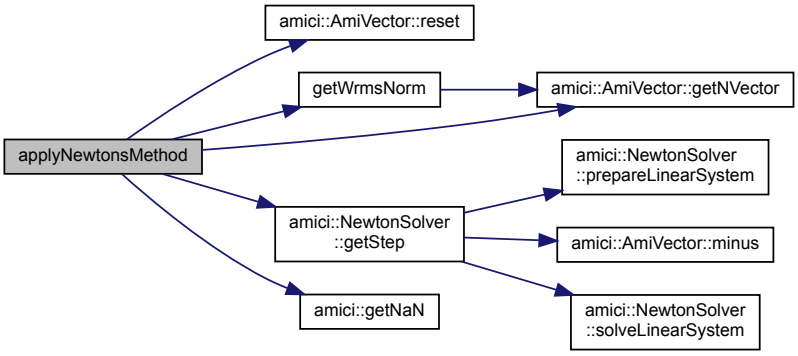
Runs the Newton solver iterations and checks for convergence to steady state

Parameters

rdata	pointer to the return data object
model	pointer to the AMICI model object
newtonSolver	pointer to the NewtonSolver object **Type**: NewtonSolver
newton_try	integer start number of Newton solver (1 or 2)

Definition at line 131 of file steadystateproblem.cpp.

Here is the call graph for this function:



10.36.3.5 writeNewtonOutput()

```
void writeNewtonOutput (
            ReturnData * rdata,
            const Model * model,
            NewtonStatus newton_status,
            double run_time,
            int it )
```

Stores output of workSteadyStateProblem in return data

Parameters

newton_status	integer flag indicating when a steady state was found
run_time	double coputation time of the solver in milliseconds
rdata	pointer to the return data instance
model	pointer to the model instance
it	current timepoint index, <0 indicates preequilibration

Definition at line 220 of file steadystateproblem.cpp.

10.36.3.6 getSteadystateSimulation()

```
void getSteadystateSimulation (
            ReturnData * rdata,
            Solver * solver,
            Model * model,
            int it )
```

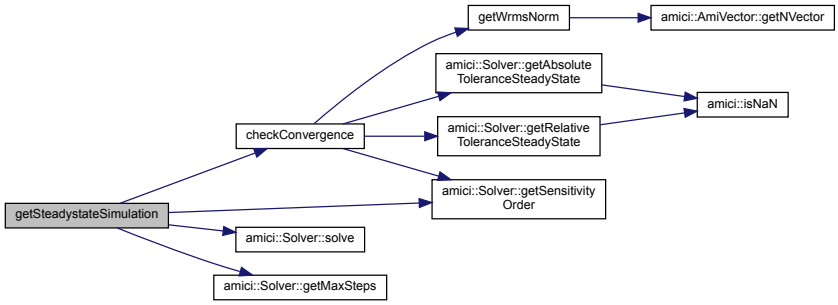
Forward simulation is launched, if Newton solver fails in first try

Parameters

solver	pointer to the AMICI solver object
model	pointer to the AMICI model object
rdata	pointer to the return data object
it	current timepoint index, <0 indicates preequilibration

Definition at line 245 of file steadystateproblem.cpp.

Here is the call graph for this function:



10.36.3.7 createSteadystateSimSolver()

```
std::unique_ptr< Solver > createSteadystateSimSolver (
            Solver * solver,
            Model * model,
            realtype tstart )
```

initialize CVodeSolver instance for preequilibration simulation

Parameters

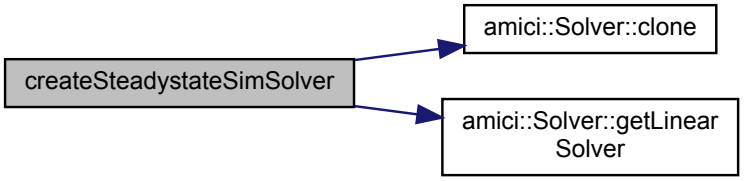
solver	pointer to the AMICI solver object
model	pointer to the AMICI model object
tstart	time point for starting Newton simulation

Returns

solver instance

Definition at line 273 of file steadystateproblem.cpp.

Here is the call graph for this function:



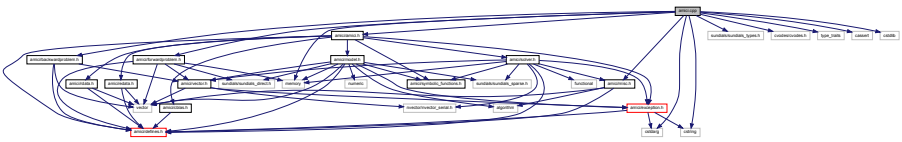
11 File Documentation

11.1 amici.cpp File Reference

core routines for integration

```
#include "amici/amici.h"
#include "amici/backwardproblem.h"
#include "amici/forwardproblem.h"
#include "amici/misc.h"
#include <sundials/sundials_types.h>
#include <cvodes/cvodes.h>
#include <type_traits>
#include <cassert>
#include <cstdlib>
#include <cstring>
#include <cstdarg>
#include <memory>
```

Include dependency graph for amici.cpp:



Namespaces

- amici

  The AMICI Python module (in doxygen this will also contain documentation about the C++ library)

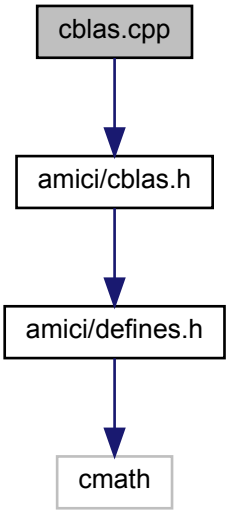
Functions

- std::unique_ptr< ReturnData > runAmiciSimulation (Solver &solver, const ExpData *edata, Model &model)
- void printErrMsgIdAndTxt (const char *identifier, const char *format,...)
- void printWarnMsgIdAndTxt (const char *identifier, const char *format,...)
- std::vector< std::unique_ptr< ReturnData > > runAmiciSimulations (Solver const &solver, const std::vector< ExpData *> &edatas, Model const &model, int num_threads)

11.2 cblas.cpp File Reference

BLAS routines required by AMICI.

`#include "amici/cblas.h"`
Include dependency graph for cblas.cpp:



Namespaces

- amici

  The AMICI Python module (in doxygen this will also contain documentation about the C++ library)

Functions

- void amici_dgemm (BLASLayout layout, BLASTranspose TransA, BLASTranspose TransB, const int M, const int N, const int K, const double alpha, const double *A, const int lda, const double *B, const int ldb, const double beta, double *C, const int ldc)
- void amici_dgemv (BLASLayout layout, BLASTranspose TransA, const int M, const int N, const double alpha, const double *A, const int lda, const double *X, const int incX, const double beta, double *Y, const int incY)
- void amici_daxpy (int n, double alpha, const double *x, const int incx, double *y, int incy)

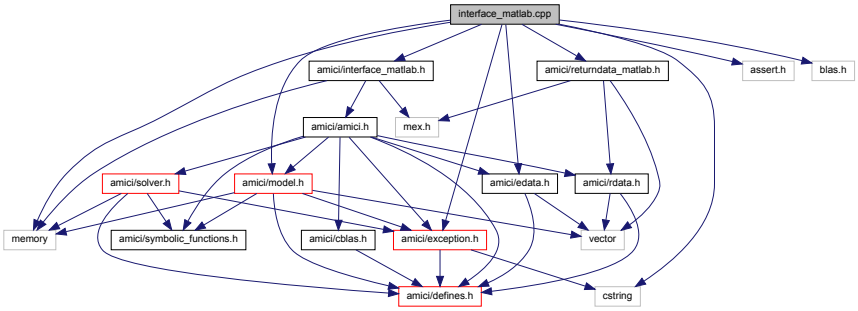
  *Compute y = a*x + y.*

11.3 interface_matlab.cpp File Reference

core routines for mex interface

```
#include "amici/interface_matlab.h"
#include "amici/model.h"
#include "amici/exception.h"
#include "amici/edata.h"
#include "amici/returndata_matlab.h"
#include <assert.h>
#include <blas.h>
#include <cstring>
#include <memory>
```

Include dependency graph for interface_matlab.cpp:



Namespaces

- amici

  The AMICI Python module (in doxygen this will also contain documentation about the C++ library)

Enumerations

- enum mexRhsArguments {
  RHS_TIMEPOINTS, **RHS_PARAMETERS**, **RHS_CONSTANTS**, **RHS_OPTIONS**, **RHS_PLIST**, **RHS_XSCALE_UNUSED**, **RHS_INITIALIZATION**, **RHS_DATA**, **RHS_NUMARGS_REQUIRED** = RHS_DATA, **RHS_NUMARGS** }

  The mexFunctionArguments enum takes care of the ordering of mex file arguments (indexing in prhs)

Functions

- int dbl2int (const double x)
- char amici_blasCBlasTransToBlasTrans (BLASTranspose trans)
- void amici_dgemm (BLASLayout layout, BLASTranspose TransA, BLASTranspose TransB, const int M, const int N, const int K, const double alpha, const double ∗A, const int lda, const double ∗B, const int ldb, const double beta, double ∗C, const int ldc)
- void amici_dgemv (BLASLayout layout, BLASTranspose TransA, const int M, const int N, const double alpha, const double ∗A, const int lda, const double ∗X, const int incX, const double beta, double ∗Y, const int incY)
- void amici_daxpy (int n, double alpha, const double ∗x, const int incx, double ∗y, int incy)

  Compute y = a∗x + y.

- std::vector< realtype > mxArrayToVector (const mxArray *array, int length)
- std::unique_ptr< ExpData > expDataFromMatlabCall (const mxArray *prhs[], const Model &model)
- void setSolverOptions (const mxArray *prhs[], int nrhs, Solver &solver)

  setSolverOptions solver options from the matlab call to a solver object
- void setModelData (const mxArray *prhs[], int nrhs, Model &model)

  setModelData sets data from the matlab call to the model object
- void mexFunction (int nlhs, mxArray *plhs[], int nrhs, const mxArray *prhs[])

11.3.1 Detailed Description

This file defines the fuction mexFunction which is executed upon calling the mex file from matlab

11.3.2 Function Documentation

11.3.2.1 mexFunction()

```
void mexFunction (
            int nlhs,
            mxArray * plhs[],
            int nrhs,
            const mxArray * prhs[] )
```

mexFunction is the main interface function for the MATLAB interface. It reads in input data (udata and edata) and creates output data compound (rdata) and then calls the AMICI simulation routine to carry out numerical integration.

Parameters

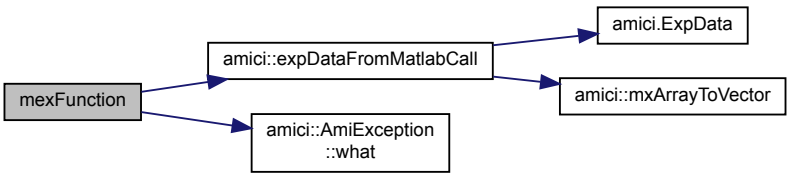
nlhs	number of output arguments of the matlab call
plhs	pointer to the array of output arguments
nrhs	number of input arguments of the matlab call
prhs	pointer to the array of input arguments

Returns

void

Definition at line 525 of file interface_matlab.cpp.

Here is the call graph for this function:



11.4 spline.cpp File Reference

definition of spline functions

Namespaces

- amici

  The AMICI Python module (in doxygen this will also contain documentation about the C++ library)

Functions

- int spline (int n, int end1, int end2, double slope1, double slope2, double x[ ], double y[ ], double b[ ], double c[ ], double d[ ])
- double seval (int n, double u, double x[ ], double y[ ], double b[ ], double c[ ], double d[ ])

  Evaluate the cubic spline function.
- double sinteg (int n, double u, double x[ ], double y[ ], double b[ ], double c[ ], double d[ ])

11.4.1 Detailed Description

Author

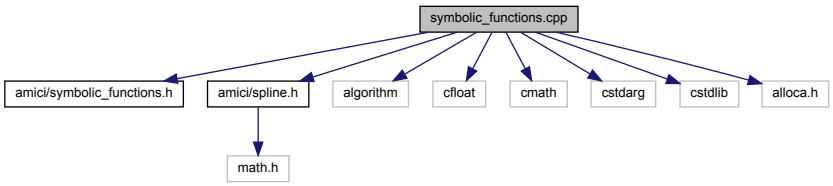
Peter & Nigel, Design Software, 42 Gubberley St, Kenmore, 4069, Australia.

11.5 symbolic_functions.cpp File Reference

definition of symbolic functions

```
#include "amici/symbolic_functions.h"
#include "amici/spline.h"
#include <algorithm>
#include <cfloat>
#include <cmath>
#include <cstdarg>
#include <cstdlib>
#include <alloca.h>
```

Include dependency graph for symbolic_functions.cpp:



Namespaces

- amici

  The AMICI Python module (in doxygen this will also contain documentation about the C++ library)

Functions

- int isNaN (double what)
- int isInf (double what)
- double getNaN ()
- double log (double x)
- double dirac (double x)
- double heaviside (double x)
- double sign (double x)
- double max (double a, double b, double c)
- double min (double a, double b, double c)
- double Dmax (int id, double a, double b, double c)
- double Dmin (int id, double a, double b, double c)
- double pos_pow (double base, double exponent)
- double spline (double t, int num,...)
- double spline_pos (double t, int num,...)
- double Dspline (int id, double t, int num,...)
- double Dspline_pos (int id, double t, int num,...)
- double DDspline (int id1, int id2, double t, int num,...)
- double DDspline_pos (int id1, int id2, double t, int num,...)

11.5.1 Detailed Description

This file contains definitions of various symbolic functions which

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