AMICI

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1 AMICI 0.1 General Documentation

1.1 Introduction

AMICI is a MATLAB interface for the SUNDIALS solvers CVODES (for ordinary differential equations) and IDAS (for algebraic differential equations). AMICI allows the user to specify differential equation models in terms of symbolic variables in MATLAB and automatically compiles such models as .mex simulation files. In contrast to the SUNDIALSTB interface, all necessary functions are transformed into native C code, which allows for a significantly faster numerical integration. Beyond forward integration, the compiled simulation file also allows for first and second order 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.

1.2 Availability

The sources for AMICI are accessible as

- Source tarball
- Source zipball
- GIT repository on github

Once you've obtained your copy check out the Installation

1.2.1 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/FFroehlich/AMICI and a direct clone is possible via

```
git clone https://github.com/FFroehlich/AMICI.git AMICI
```

1.2.2 License Conditions

This software is available under the BSD license

1.3 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.

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

```
installToolbox.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.de

The tools SUNDIALS and SuiteSparse shipped with AMICI do **not** require further 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

2 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 `master`
- Implement your changes
- Submit a pull request
- Make sure your code is documented appropriately
- 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 got broken
  - Run `tests/cpputest/wrapTestModels.m` followed by CI tests `scripts/run-build.sh && scripts/run-cpputest.sh`
  - Run `examples/amiExamples.m`
- When all tests are passing and you think your code is ready to merge, request a code review

3 SBMLimporter

MATLAB toolbox to generate ODE models from SBML files

4 Model Definition & Simulation

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

4.1 Model Definition

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

4.1.1 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()
```

4.1.2 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	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 true, the fields 'noforward' and 'noadjoint' will speed up the time required to compile the model but also disable the respective sensitivity computation.

4.1.3 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:

```
x = [ state1 state2 state3 ];
```

4.1.4 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

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

4.1.5 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

```
k = [ const1 const2 ];
```

4.1.6 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

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

or

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

The specification of f or xdot may depend on States, Parameters and Constants.

For DAEs also specify the mass matrix.

```
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 symbolic_functions.c.

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.

4.1.7 Initial Conditions

Specify the initial conditions. These may depend on Parameters on Constants and must have the same size as x.

```
x0 = [ param4, 0, 0 ];
```

4.1.8 Observables

Specify the observables. These may depend on Parameters and Constants.

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

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

4.1.9 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.

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

Events may depend on States, Parameters and Constants but **not** on Observables

4.1.10 Standard Deviation

Specifying of 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

```
sigma_y(1) = param5;
```

Standard deviaton for event data is denoted by sigma_y

```
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 Sigma_Y or Sigma_T in the user-provided data struct is NaN. See Model Simulation for details.

4.1.11 Attach to Model Struct

Eventually all symbolic expressions need to be attached to the model struct.

```
model.sym.x = x;
model.sym.k = k;
model.sym.event = event;
model.sym.xdot = xdot;
% or
model.sym.f = f;
model.sym.M = M; %only for DAEs
model.sym.p = p;
model.sym.x0 = x0;
model.sym.y = y;
model.sym.sigma_y = sigma_y;
model.sym.sigma_t = sigma_t;
```

4.2 Model Compilation

The model can then be compiled by calling amiwrap:

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

Here modelname should be a string defining the modelname, 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 model and pass them directly to amiwrap() without generating respective model definition scripts.

See also

amiwrap()

4.3 Model Simulation

After the call to amiwrap() two files will be placed in the specified directory. One is a am_*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.

4.3.1 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 events will then be available as sol.root. 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.rval.

Alternatively the integration call also be called via

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

The integration status will be indicated by the status flag. 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.

4.3.2 Forward Sensitivities

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);
```

Set the sensitivity computation to forward sensitivities and Integrate:

```
options.sensi = 1;
options.forward = true;
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, with the derivative with respect to the parameters in sol.sx. The observables will then be available as sol.y, with the derivative with respect to the parameters in sol.sy. The events will then be available as sol.root, with the derivative with respect to the parameters in sol.sroot. 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.rootval, with the derivative with respect to the parameters in sol.srootval

Alternatively the integration call 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 indicated 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.

4.3.3 Adjoint Sensitivities

Define a time vector:

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

Generate a parameter vector:

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

Set the sensitivity computation to adjoint sensitivities:

```
options.sensi = 1;
options.adjoint = true;
```

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 Standard Deviation. Data points with NaN value will be completely ignored.

Generate a constants vector:

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

Integrate:

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

The integration status will be indicated by the sol.status flag. Negative values indicated 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.

4.3.4 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.

Define a final timepoint t:

```
t = 100
```

Generate a parameter vector:

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

Generate a constants vector:

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

Set the sensitivity computation to steady state sensitivities:

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

Integrate:

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

The states will then be available as sol.x, with the derivative with respect to the parameters in sol.sx. The observables will then 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.xdot.

5 Code Organization

In the following we will briefly outline what happens when a model is compiled. For a more detailed description we refer the reader to the documentation of the individual functions.

After specifying a model (see Model Definition) the user will typically compile the model by invoking amiwrap(). amiwrap() first instantiates an object of the class amimodel. The properties of this object are initialised based on the user-defined model. If the o2flag is active, all subsequent computations will also be carried out on the augmented system, which also includes the equations for forward sensitivities. This allows the computation of second order sensitivities in a forward-forward approach. A forward-adjoint approach will be implemented in the future.

The fun fields of this object will then be populated by amimodel::parseModel(). The amimodel::fun field contains all function definitions of type amifun which are required for model compilation. The set of functions to be considered will depend on the user specification of the model fields amimodel::adjoint and amimodel::forward (see Options) as well as the employed solver (CVODES or IDAS, see Differential Equation). For all considered functions amimodel::parseModel() will check their dependencies via amimodel::checkDeps(). These dependencies are a subset of the user-specified fields of amimodel::fun (see Attach to Model Struct). amimodel::parseModel() compares the hashes of all dependencies against the amimodel::HTable of possible previous compilations and will only compute necessary symbolic expressions if changes in these fields occured.

For all functions for which amimodel::fun exists, amimodel::generateC() will generate C files. These files together with their respective header files will be placed in $AMICIDIR/models/*modelname*. amimodel::generateC() will also generate wrapfunctions.h and wrapfunctions.c. These files define and declare model unspecific wrapper functions around model specific functions. This construction allows us to use to build multiple different models against the same simulation routines by linking different realisations of these wrapper functions.

All the generated C functions are subsequently compiled by amimodel::compileC(). For all functions individual object files are created to reduce the computation cost of code optimization. Moreover necessary code from sundials and SuiteSparse is compiled as object files and placed in /models/*mexext*, where mexext stands for the string returned by matlab to the command mexext. The mex simulation file is compiled from amiwrap.c, linked against all object necessary of sundials, SuiteSparse and model specific functions. Depending on the required solver, the compilation will either include cvodewrap.h or idawrap.h. These files implement solver specific realisations of the AMI... functions used in amiwrap.c and amici.c. This allows the use of the same simulation routines for both CVODES and IDAS.

6 Using AMICI-generated code outside Matlab

AMICI (amiwrap.m) translates the model definition into C++ code which is then compiled into a mex file for MATLAB. Advanced users can use this code within stand-online C/C++ applications for use in non-MATLAB 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 usually 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
model_steadystate_deltaqB_mexa64.md5
model_steadystate_deltaqB.o
[... many more files model_steadystate_*.(cpp|h|md5|o) ]
wrapfunctions.cpp
wrapfunctions.h
wrapfunctions.o
```

Only `*.cpp` and `*.h` files will be needed for the model; `*.o` and `*.md5` are not required.

Running a simulation

The entry function for running an AMICI simulation is getSimulationResults(), declared in amici.h. This function requires all AMICI options and any experimental data. All options that would normally be passed to `simulate_${MODEL_NAME}()` in MATLAB are passed in a UserData struct (see `udata.h` for info). Any experimental data will be passed as ExpData struct (`edata.h`). The simulation results will be returned in a ReturnData struct (see `rdata.h`).

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. (There are some accessor macro definitions available in udata_accessors.h, rdata_accessors.h and edata_accessors.h which provide shortcuts for accessing struct members of UserData, ReturnData, ExpData, respectively. `amici_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/*.c`
the SUNDIALS and the SUITESPARSE library.

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`. (NOTE: This sample program should compile and link, but will crash most certainly without further problem-specific adaptations.)

7 Hierarchical Index

7.1 Class Hierarchy

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

8 Class Index

8.1 Class List

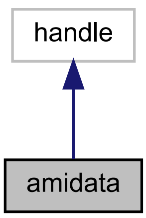
Here are the classes, structs, unions and interfaces with brief descriptions:

9 Class Documentation

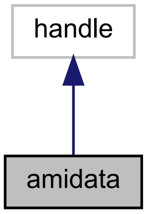
9.1 amidata Class Reference

AMIDATA provides a data container to pass experimental data to the simulation routine for likelihood computation. when any of the properties are updated, the class automatically checks consistency of dimension and updates related properties and initialises them with NaNs.

Inheritance diagram for amidata:



Collaboration diagram for amidata:



Public Member Functions

- amidata (matlabtypesubstitute varargin)

  amidata creates an container for experimental data with specified dimensions amidata.

Public Attributes

- matlabtypesubstitute nt = 0

  number of timepoints
- matlabtypesubstitute ny = 0

  number of observables
- matlabtypesubstitute nz = 0

  number of event observables
- matlabtypesubstitute ne = 0

  number of events
- matlabtypesubstitute nk = 0

  number of conditions/constants
- matlabtypesubstitute t = double.empty("")

  timepoints of observations
- matlabtypesubstitute Y = double.empty("")

  observations
- matlabtypesubstitute Sigma_Y = double.empty("")

  standard deviation of observations
- matlabtypesubstitute Z = double.empty("")

  event observations
- matlabtypesubstitute Sigma_Z = double.empty("")

  standard deviation of event observations
- matlabtypesubstitute condition = double.empty("")

  experimental condition

9.1.1 Detailed Description

Definition at line 17 of file amidata.m.

9.1.2 Constructor & Destructor Documentation

9.1.2.1 amidata()

```
amidata (
          matlabtypesubstitute varargin )
```

AMIDATA(amidata) creates a copy of the input container

AMIDATA(struct) tries to creates an amidata container from the input struct. the struct should have the following

fields

t [nt,1] Y [nt,ny] Sigma_Y [nt,ny] Z [ne,nz] Sigma_Z [ne,nz] condition [nk,1]

if some fields are missing the function will try to initialise them with NaNs with consistent dimensions

AMIDATA(nt,ny,nz,ne,nk) constructs an empty data container with in the provided dimensions intialised with NaNs

Parameters

varargin	

Definition at line 122 of file amidata.m.

9.1.3 Member Data Documentation

9.1.3.1 nt

```
nt = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 31 of file amidata.m.

9.1.3.2 ny

```
ny = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 39 of file amidata.m.

9.1.3.3 nz

```
nz = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 47 of file amidata.m.

9.1.3.4 ne

```
ne = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 55 of file amidata.m.

9.1.3.5 nk

```
nk = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 63 of file amidata.m.

9.1.3.6 t

```
t = double.empty("")
```

Default: double.empty("")

Note

This property has custom functionality when its value is changed.

Definition at line 71 of file amidata.m.

9.1.3.7 Y

```
Y = double.empty("")
```

Default: double.empty("")

Note

This property has custom functionality when its value is changed.

Definition at line 79 of file amidata.m.

9.1.3.8 Sigma_Y

```
Sigma_Y = double.empty("")
```

Default: double.empty("")

Note

This property has custom functionality when its value is changed.

Definition at line 87 of file amidata.m.

9.1.3.9 Z

```
Z = double.empty("")
```

Default: double.empty("")

Note

This property has custom functionality when its value is changed.

Definition at line 95 of file amidata.m.

9.1.3.10 Sigma_Z

```
Sigma_Z = double.empty("")
```

Default: double.empty("")

Note

This property has custom functionality when its value is changed.

Definition at line 103 of file amidata.m.

9.1.3.11 condition

```
condition = double.empty("")
```

Default: double.empty("")

Note

This property has custom functionality when its value is changed.

Definition at line 111 of file amidata.m.

9.2 amievent Class Reference

AMIEVENT defines events which later on will be transformed into appropriate C code.

Public Member Functions

- amievent (matlabtypesubstitute trigger, matlabtypesubstitute bolus, matlabtypesubstitute z)

  amievent constructs an amievent object from the provided input.
- mlhsInnerSubst< matlabtypesubstitute > setHflag (::double hflag)

  gethflag sets the hflag property.

Public Attributes

- ::symbolic trigger = sym.empty("")

  the trigger function activates the event on every zero crossing
- ::symbolic bolus = sym.empty("")

  the bolus function defines the change in states that is applied on every event occurence
- ::symbolic z = sym.empty("")

  output function for the event
- matlabtypesubstitute hflag = logical.empty("")

  flag indicating that a heaviside function is present, this helps to speed up symbolic computations

9.2.1 Detailed Description

Definition at line 17 of file amievent.m.

9.2.2 Constructor & Destructor Documentation

9.2.2.1 amievent()

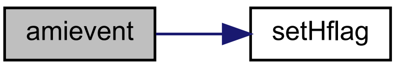
```
amievent (
            matlabtypesubstitute trigger,
            matlabtypesubstitute bolus,
            matlabtypesubstitute z )
```

Parameters

trigger	trigger function, the event will be triggered on at all roots of this function
bolus	the bolus that will be added to all states on every occurence of the event
z	the event output that will be reported on every occurence of the event

Definition at line 75 of file amievent.m.

Here is the call graph for this function:



9.2.3 Member Function Documentation

9.2.3.1 setHflag()

```
mlhsInnerSubst<::amievent > setHflag (
            ::double hflag )
```

Parameters

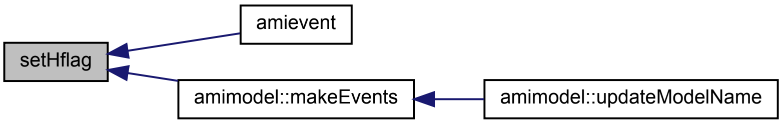
hflag	value for the hflag property

Return values

this	updated event definition object

Definition at line 18 of file setHflag.m.

Here is the caller graph for this function:



9.2.4 Member Data Documentation

9.2.4.1 trigger

```
trigger = sym.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: sym.empty("")

Definition at line 27 of file amievent.m.

9.2.4.2 bolus

```
bolus = sym.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: sym.empty("")

Definition at line 38 of file amievent.m.

9.2.4.3 z

```
z = sym.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: sym.empty("")

Definition at line 49 of file amievent.m.

9.2.4.4 hflag

```
hflag = logical.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: logical.empty("")

Definition at line 60 of file amievent.m.

9.3 amifun Class Reference

AMIFUN defines functions which later on will be transformed into appropriate C code.

Public Member Functions

- amifun (matlabtypesubstitute funstr, matlabtypesubstitute model)
  amievent constructs an amifun object from the provided input.
- noret::substitute printLocalVars (::amimodel model,::fileid fid)
  printlocalvars prints the C code for the initialisation of local variables into the file specified by fid.
- noret::substitute writeCcode_sensi (::amimodel model,::fileid fid)
  writeCcode_sensi is a wrapper for writeCcode which loops over parameters and reduces overhead by check nonzero values
- noret::substitute writeCcode (::amimodel model,::fileid fid)
  writeCcode is a wrapper for gccode which initialises data and reduces overhead by check nonzero values
- noret::substitute writeMcode (::amimodel model)
  writeMcode generates matlab evaluable code for specific model functions
- noret::substitute gccode (::amimodel model,::fileid fid)
  gccode transforms symbolic expressions into c code and writes the respective expression into a specified file
- mlhsInnerSubst$<$ matlabtypesubstitute $>$ getDeps (::amimodel model)
  getDeps populates the sensiflag for the requested function
- mlhsInnerSubst$<$ matlabtypesubstitute $>$ getArgs (::amimodel model)

getFArgs populates the fargstr property with the argument string of the respective model function (if applicable). model functions are not wrapped versions of functions which have a model specific name and for which the call is solver specific.

- mlhsInnerSubst< matlabtypesubstitute > getFArgs ()

  getFArgs populates the fargstr property with the argument string of the respective f-function (if applicable). f-function are wrapped implementations of functions which no longer have a model specific name and have solver independent calls.

- mlhsInnerSubst< matlabtypesubstitute > getNVecs ()

  getfunargs populates the nvecs property with the names of the N_Vector elements which are required in the execution of the function (if applicable). the information is directly extracted from the argument string

- mlhsInnerSubst< matlabtypesubstitute > getCVar ()

  getCVar populates the cvar property

- mlhsInnerSubst< matlabtypesubstitute > getSensiFlag ()

  getSensiFlag populates the sensiflag property

Public Attributes

- ::symbolic sym = sym("[ ]")

  symbolic definition struct

- ::symbolic sym_noopt = sym("[ ]")

  symbolic definition which was not optimized (no dependencies on w)

- ::symbolic strsym = sym("[ ]")

  short symbolic string which can be used for the reuse of precomputed values

- ::symbolic strsym_old = sym("[ ]")

  short symbolic string which can be used for the reuse of old values

- ::char funstr = char.empty("")

  name of the model

- ::char cvar = char.empty("")

  name of the c variable

- ::char argstr = char.empty("")

  argument string (solver specific)

- ::char fargstr = char.empty("")

  argument string (solver unspecific)

- ::cell deps = cell.empty("")

  dependencies on other functions

- matlabtypesubstitute nvecs = cell.empty("")

  nvec dependencies

- matlabtypesubstitute sensiflag = logical.empty("")

  indicates whether the function is a sensitivity or derivative with respect to parameters

9.3.1 Detailed Description

Definition at line 17 of file amifun.m.

9.3.2 Constructor & Destructor Documentation

9.3.2.1 amifun()

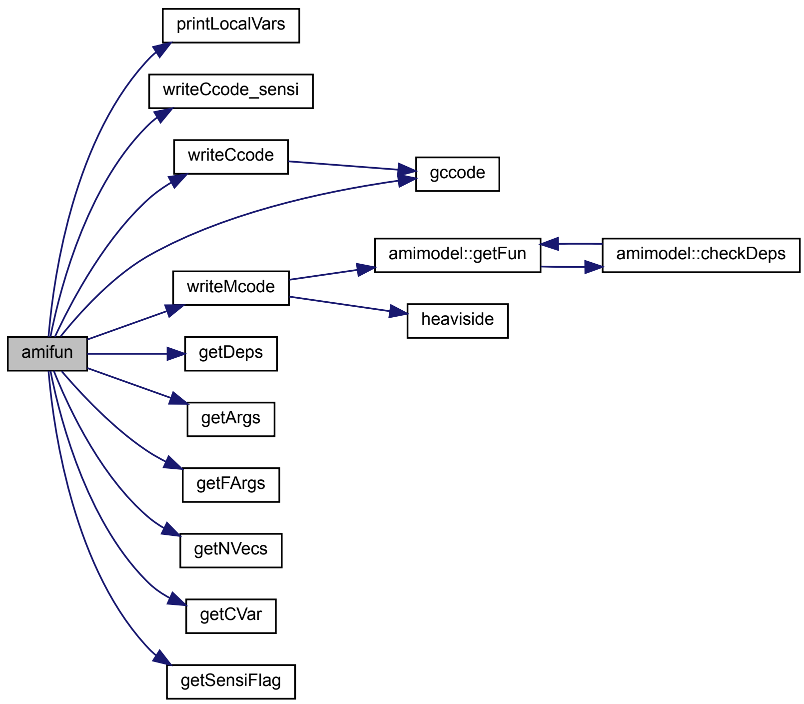
```
amifun (
        matlabtypesubstitute funstr,
        matlabtypesubstitute model )
```

Parameters

funstr	name of the requested function
model	amimodel object which carries all symbolic definitions to construct the function

Definition at line 119 of file amifun.m.

Here is the call graph for this function:



9.3.3 Member Function Documentation

9.3.3.1 printLocalVars()

```
noret::substitute printLocalVars (
            ::amimodel model,
            ::fileid fid )
```

Parameters

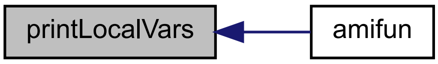
model	this struct must contain all necessary symbolic definitions
fid	file id in which the final expression is written

Return values

fid	Nothing

Definition at line 18 of file printLocalVars.m.

Here is the caller graph for this function:



9.3.3.2 writeCcode_sensi()

```
noret::substitute writeCcode_sensi (
            ::amimodel model,
            ::fileid fid )
```

Parameters

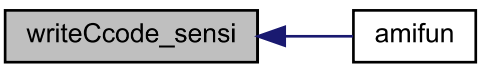
model	model defintion object
fid	file id in which the final expression is written

Return values

fid	void

Definition at line 18 of file writeCcode_sensi.m.

Here is the caller graph for this function:



9.3.3.3 writeCcode()

```
noret::substitute writeCcode (
              ::amimodel model,
              ::fileid fid )
```

Parameters

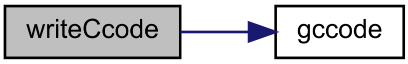
model	model defintion object
fid	file id in which the final expression is written

Return values

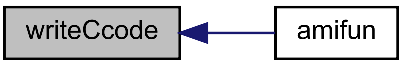
fid	void

Definition at line 18 of file writeCcode.m.

Here is the call graph for this function:



Here is the caller graph for this function:



9.3.3.4 writeMcode()

```
noret::substitute writeMcode (
              ::amimodel model )
```

Parameters

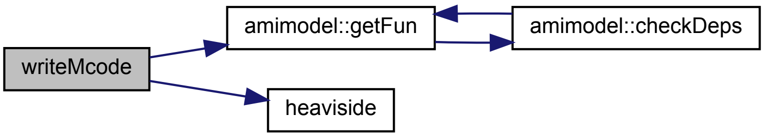
model	model defintion object

Return values

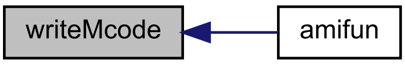
model	void

Definition at line 18 of file writeMcode.m.

Here is the call graph for this function:



Here is the caller graph for this function:



9.3.3.5 gccode()

```
mlhsInnerSubst<::amifun > gccode (
              ::amimodel model,
              ::fileid fid )
```

Parameters

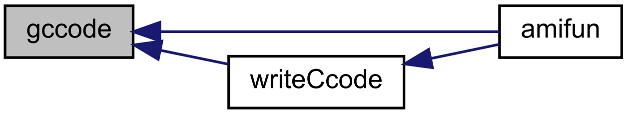
model	model definition object
fid	file id in which the expression should be written

Return values

this	function definition object

Definition at line 18 of file gccode.m.

Here is the caller graph for this function:



9.3.3.6 getDeps()

```
mlhsInnerSubst<::amifun > getDeps (
              ::amimodel model )
```

Parameters

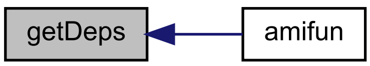
model	model definition object

Return values

this	updated function definition object

Definition at line 18 of file getDeps.m.

Here is the caller graph for this function:



9.3.3.7 getArgs()

```
mlhsInnerSubst<::amifun > getArgs (
              ::amimodel model )
```

Parameters

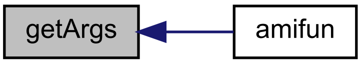
model	model definition object

Return values

this	updated function definition object

Definition at line 18 of file getArgs.m.

Here is the caller graph for this function:



9.3.3.8 getFArgs()

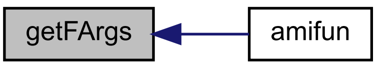
```
mlhsInnerSubst<::amifun > getFArgs ( )
```

Return values

this	updated function definition object

Definition at line 18 of file getFArgs.m.

Here is the caller graph for this function:



9.3.3.9 getNVecs()

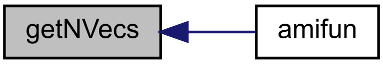
```
mlhsInnerSubst<::amifun > getNVecs ( )
```

Return values

this	updated function definition object

Definition at line 18 of file getNVecs.m.

Here is the caller graph for this function:



9.3.3.10 getCVar()

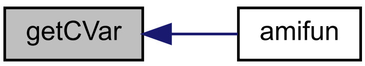
`mlhsInnerSubst<::amifun > getCVar ( )`

Return values

this	updated function definition object

Definition at line 18 of file getCVar.m.

Here is the caller graph for this function:



9.3.3.11 getSensiFlag()

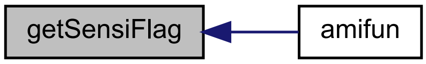
`mlhsInnerSubst<::amifun > getSensiFlag ( )`

Return values

this	updated function definition object

Definition at line 18 of file getSensiFlag.m.

Here is the caller graph for this function:



9.3.4 Member Data Documentation

9.3.4.1 sym

```
sym = sym("[]")
```

Default: sym("[]")

Definition at line 27 of file amifun.m.

9.3.4.2 sym_noopt

```
sym_noopt = sym("[]")
```

Default: sym("[]")

Definition at line 35 of file amifun.m.

9.3.4.3 strsym

```
strsym = sym("[]")
```

Default: sym("[]")

Definition at line 43 of file amifun.m.

9.3.4.4 strsym_old

```
strsym_old = sym("[]")
```

Default: sym("[]")

Definition at line 51 of file amifun.m.

9.3.4.5 funstr

```
funstr = char.empty("")
```

Default: char.empty("")

Definition at line 59 of file amifun.m.

9.3.4.6 cvar

```
cvar = char.empty("")
```

Default: char.empty("")

Definition at line 67 of file amifun.m.

9.3.4.7 argstr

```
argstr = char.empty("")
```

Default: char.empty("")

Definition at line 75 of file amifun.m.

9.3.4.8 fargstr

```
fargstr = char.empty("")
```

Default: char.empty("")

Definition at line 83 of file amifun.m.

9.3.4.9 deps

```
deps = cell.empty("")
```

Default: cell.empty("")

Definition at line 91 of file amifun.m.

9.3.4.10 nvecs

```
nvecs = cell.empty("")
```

Default: cell.empty("")

Definition at line 99 of file amifun.m.

9.3.4.11 sensiflag

```
sensiflag = logical.empty("")
```

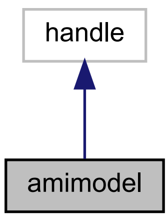
Default: logical.empty("")

Definition at line 107 of file amifun.m.

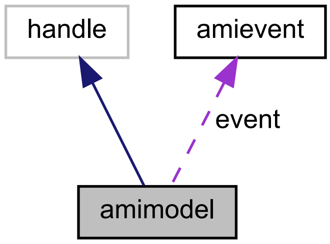
9.4 amimodel Class Reference

AMIMODEL carries all model definitions including functions and events.

Inheritance diagram for amimodel:



Collaboration diagram for amimodel:



Public Member Functions

- amimodel (::string symfun,::string modelname)

  amimodel initializes the model object based on the provided symfun and modelname
- noret::substitute updateRHS (matlabtypesubstitute xdot)

  updateRHS updates the private fun property .fun.xdot.sym (right hand side of the differential equation)
- noret::substitute updateModelName (matlabtypesubstitute modelname)

  updateModelName updates the modelname
- noret::substitute parseModel ()

  parseModel parses the model definition and computes all necessary symbolic expressions.
- noret::substitute generateC ()

  generateC generates the c files which will be used in the compilation.
- noret::substitute compileC ()

  compileC compiles the mex simulation file
- noret::substitute generateM (::amimodel amimodelo2)

  generateM generates the matlab wrapper for the compiled C files.
- noret::substitute getFun (::struct HTable,::string funstr)

  getFun generates symbolic expressions for the requested function.
- noret::substitute makeEvents ()

  makeEvents extracts discontiniuties from the model right hand side and converts them into events
- noret::substitute makeSyms ()

  makeSyms extracts symbolic definition from the user provided model and checks them for consistency
- mlhsInnerSubst< matlabtypesubstitute > checkDeps (::struct HTable,::cell deps)

  checkDeps checks the dependencies of functions and populates sym fields if necessary
- mlhsInnerSubst< matlabtypesubstitute > loadOldHashes ()

  loadOldHashes loads information from a previous compilation of the model.
- mlhsInnerSubst< matlabtypesubstitute > augmento2 ()

  augmento2 augments the system equation to also include equations for sensitivity equation. This will enable us to compute second order sensitivities in a forward-adjoint or forward-forward apporach later on.
- mlhsInnerSubst< matlabtypesubstitute > augmento2vec ()

  augmento2 augments the system equation to also include equations for sensitivity equation. This will enable us to compute second order sensitivities in a forward-adjoint or forward-forward apporach later on.

Static Public Member Functions

- static noret::substitute compileAndLinkModel (matlabtypesubstitute modelname, matlabtypesubstitute wrap_path, matlabtypesubstitute recompile, matlabtypesubstitute coptim, matlabtypesubstitute debug, matlabtypesubstitute funs, matlabtypesubstitute cfun, matlabtypesubstitute adjoint)

  compileAndLinkModel compiles the mex simulation file. It does not check if the model files have changed since generating C++ code or whether all files are still present. Use only if you know what you are doing. The safer alternative is rerunning amiwrap().

Public Attributes

- ::struct sym = struct.empty("")

  symbolic definition struct
- ::struct fun = struct.empty("")

  struct which stores information for which functions c code needs to be generated
- ::amievent event = amievent.empty("")

  struct which stores information for which functions c code needs to be generated
- ::string modelname = char.empty("")

  name of the model
- ::struct HTable = struct.empty("")

  struct that contains hash values for the symbolic model definitions
- ::bool debug = false

  flag indicating whether debugging symbols should be compiled
- ::bool adjoint = true

  flag indicating whether adjoint sensitivities should be enabled
- ::bool forward = true

  flag indicating whether forward sensitivities should be enabled
- ::bool steadystate = true

  flag indicating whether steady state sensitivities should be enabled
- ::double t0 = 0

  default initial time
- ::string wtype = char.empty("")

  type of wrapper (cvodes/idas)
- ::int nx = double.empty("")

  number of states
- ::int nxtrue = double.empty("")

  number of original states for second order sensitivities
- ::int ny = double.empty("")

  number of observables
- ::int nytrue = double.empty("")

  number of original observables for second order sensitivities
- ::int np = double.empty("")

  number of parameters
- ::int nk = double.empty("")

  number of constants
- ::int ng = double.empty("")

  number of objective functions
- ::int nevent = double.empty("")

  number of events
- ::int nz = double.empty("")

  number of event outputs

- ::int nztrue = double.empty("")

    number of original event outputs for second order sensitivities
- ::∗int id = double.empty("")

    flag for DAEs
- ::int ubw = double.empty("")

    upper Jacobian bandwidth
- ::int lbw = double.empty("")

    lower Jacobian bandwidth
- ::int nnz = double.empty("")

    number of nonzero entries in Jacobian
- ::∗int sparseidx = double.empty("")

    dataindexes of sparse Jacobian
- ::∗int rowvals = double.empty("")

    rowindexes of sparse Jacobian
- ::∗int colptrs = double.empty("")

    columnindexes of sparse Jacobian
- ::∗int sparseidxB = double.empty("")

    dataindexes of sparse Jacobian
- ::∗int rowvalsB = double.empty("")

    rowindexes of sparse Jacobian
- ::∗int colptrsB = double.empty("")

    columnindexes of sparse Jacobian
- ::∗cell funs = cell.empty("")

    cell array of functions to be compiled
- ::∗cell mfuns = cell.empty("")

    cell array of matlab functions to be compiled
- ::string coptim = "-O3"

    optimisation flag for compilation
- ::string param = "lin"

    default parametrisation
- matlabtypesubstitute wrap_path = char.empty("")

    path to wrapper
- matlabtypesubstitute recompile = false

    flag to enforce recompilation of the model
- matlabtypesubstitute cfun = struct.empty("")

    storage for flags determining recompilation of individual functions
- matlabtypesubstitute o2flag = 0

    flag which identifies augmented models 0 indicates no augmentation 1 indicates augmentation by first order sensitivities (yields second order sensitivities) 2 indicates augmentation by one linear combination of first order sensitivities (yields hessian-vector product)
- matlabtypesubstitute z2event = double.empty("")

    vector that maps outputs to events
- matlabtypesubstitute splineflag = false

    flag indicating whether the model contains spline functions
- matlabtypesubstitute minflag = false

    flag indicating whether the model contains min functions
- matlabtypesubstitute maxflag = false

    flag indicating whether the model contains max functions
- ::int nw = 0

    number of derived variables w, w is used for code optimization to reduce the number of frequently occuring expressions

- ::int ndwdx = 0

  number of derivatives of derived variables w, dwdx
- ::int ndwdp = 0

  number of derivatives of derived variables w, dwdp

9.4.1 Detailed Description

Definition at line 17 of file amimodel.m.

9.4.2 Constructor & Destructor Documentation

9.4.2.1 amimodel()

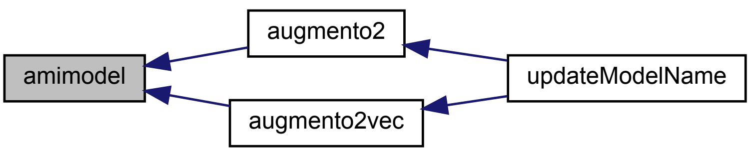
```
amimodel (
            ::string symfun,
            ::string modelname )
```

Parameters

symfun	this is the string to the function which generates the modelstruct. You can also directly pass the struct here
modelname	name of the model

Definition at line 526 of file amimodel.m.

Here is the caller graph for this function:



9.4.3 Member Function Documentation

9.4.3.1 updateRHS()

```
noret::substitute updateRHS (
            matlabtypesubstitute xdot )
```

Parameters

xdot	new right hand side of the differential equation

Definition at line 623 of file amimodel.m.

9.4.3.2 updateModelName()

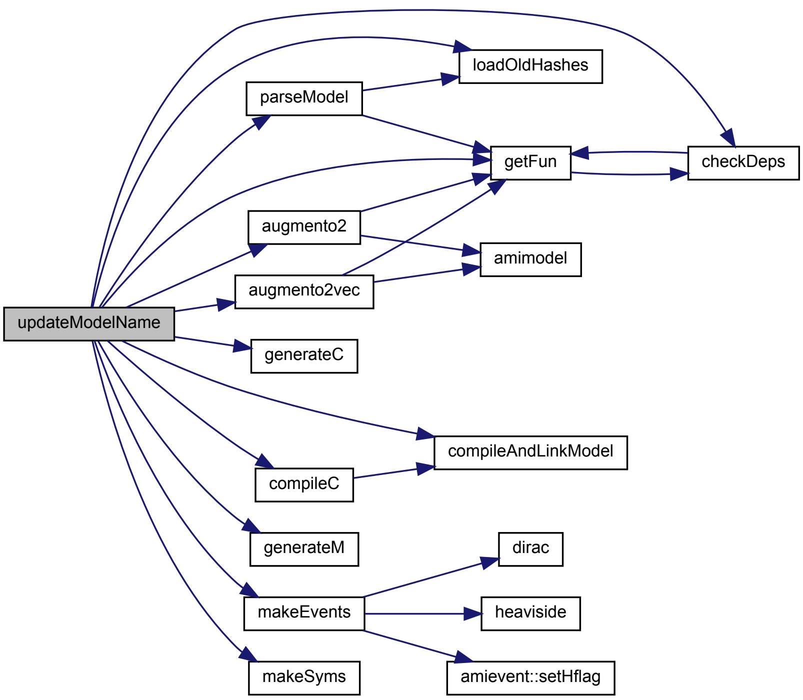
```
noret::substitute updateModelName (
            matlabtypesubstitute modelname )
```

Parameters

modelname	new modelname

Definition at line 636 of file amimodel.m.

Here is the call graph for this function:



9.4.3.3 generateC()

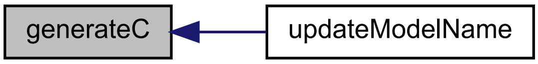
```
noret::substitute generateC ( )
```

Return values

this	model definition object

Definition at line 18 of file generateC.m.

Here is the caller graph for this function:



9.4.3.4 compileC()

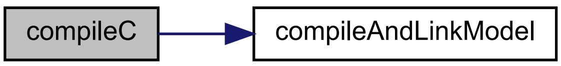
```
noret::substitute compileC ( )
```

Return values

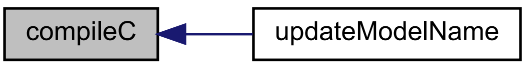
this	model definition object

Definition at line 18 of file compileC.m.

Here is the call graph for this function:



Here is the caller graph for this function:



9.4.3.5 generateM()

```
noret::substitute generateM (
            ::amimodel amimodelo2 )
```

Parameters

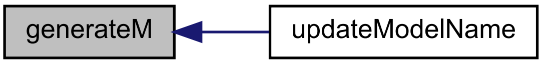
amimodelo2	this struct must contain all necessary symbolic definitions for second order sensivities

Return values

this	model definition object

Definition at line 18 of file generateM.m.

Here is the caller graph for this function:



9.4.3.6 getFun()

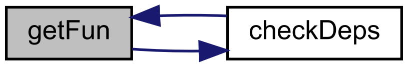
```
noret::substitute getFun (
            ::struct HTable,
            ::string funstr )
```

Parameters

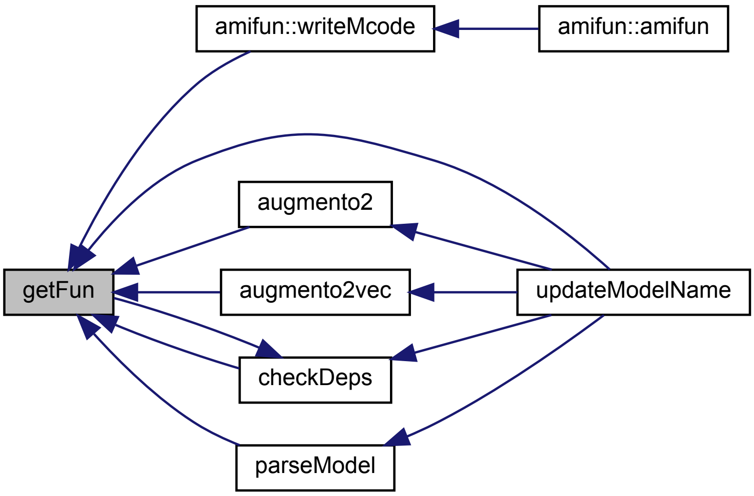
HTable	struct with hashes of symbolic definition from the previous compilation
funstr	function for which symbolic expressions should be computed

Definition at line 18 of file getFun.m.

Here is the call graph for this function:



Here is the caller graph for this function:



9.4.3.7 checkDeps()

```
mlhsInnerSubst< ::bool > checkDeps (
              ::struct HTable,
              ::cell deps )
```

Parameters

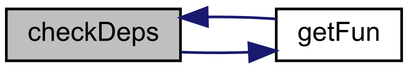
HTable	struct with reference hashes of functions in its fields
deps	cell array with containing a list of dependencies

Return values

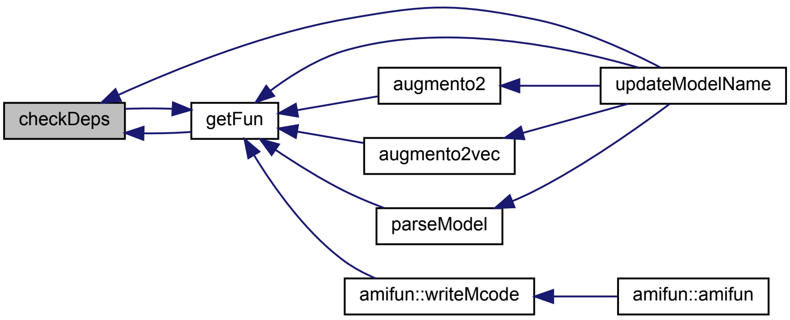
cflag	boolean indicating whether any of the dependencies have changed with respect to the hashes stored in HTable

Definition at line 18 of file checkDeps.m.

Here is the call graph for this function:



Here is the caller graph for this function:



9.4.3.8 loadOldHashes()

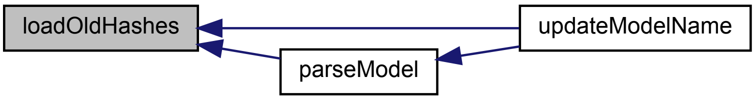
```
mlhsInnerSubst<::struct > loadOldHashes ( )
```

Return values

HTable	struct with hashes of symbolic definition from the previous compilation

Definition at line 18 of file loadOldHashes.m.

Here is the caller graph for this function:



9.4.3.9 augmento2()

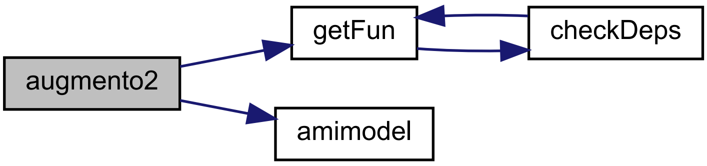
```
mlhsInnerSubst< matlabtypesubstitute > augmento2 ( )
```

Return values

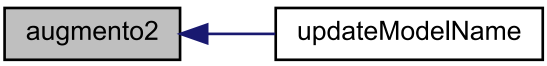
this	augmented system which contains symbolic definition of the original system and its sensitivities

Definition at line 18 of file augmento2.m.

Here is the call graph for this function:



Here is the caller graph for this function:



9.4.3.10 augmento2vec()

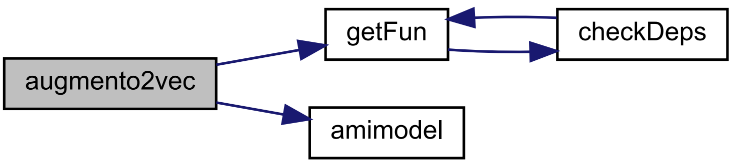
```
mlhsInnerSubst< matlabtypesubstitute > augmento2vec ( )
```

Return values

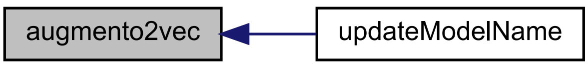
this	augmented system which contains symbolic definition of the original system and its sensitivities

Definition at line 18 of file augmento2vec.m.

Here is the call graph for this function:



Here is the caller graph for this function:



9.4.3.11 compileAndLinkModel()

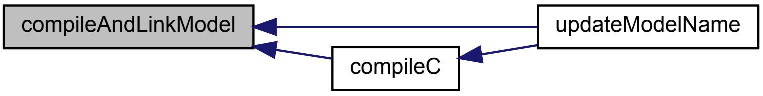
```
noret::substitute compileAndLinkModel (
            matlabtypesubstitute modelname,
            matlabtypesubstitute wrap_path,
            matlabtypesubstitute recompile,
            matlabtypesubstitute coptim,
            matlabtypesubstitute debug,
            matlabtypesubstitute funs,
            matlabtypesubstitute cfun,
            matlabtypesubstitute adjoint )  [static]
```

Parameters

modelname	name of the model as specified for amiwrap() wrap_path AMICI path recompile flag indicating whether all source files should be recompiled coptim optimization flags debug enable debugging? funs array with names of the model functions, will be guessed from source files if left empty cfun struct indicating which files should be recompiled adjoint flag indicating whether adjoint sensitivies are enabled

Definition at line 18 of file compileAndLinkModel.m.

Here is the caller graph for this function:



9.4.4 Member Data Documentation

9.4.4.1 sym

```
sym = struct.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: struct.empty("")

Definition at line 27 of file amimodel.m.

9.4.4.2 fun

```
fun = struct.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: struct.empty("")

Definition at line 38 of file amimodel.m.

9.4.4.3 event

```
event = amievent.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: amievent.empty("")

Definition at line 49 of file amimodel.m.

9.4.4.4 modelname

```
modelname = char.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: char.empty("")

Definition at line 61 of file amimodel.m.

9.4.4.5 HTable

```
HTable = struct.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: struct.empty("")

Definition at line 72 of file amimodel.m.

9.4.4.6 debug

```
debug = false
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: false

Definition at line 83 of file amimodel.m.

9.4.4.7 adjoint

`adjoint = true`

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: true

Definition at line 94 of file amimodel.m.

9.4.4.8 forward

`forward = true`

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: true

Definition at line 105 of file amimodel.m.

9.4.4.9 steadystate

`steadystate = true`

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: true

Definition at line 116 of file amimodel.m.

9.4.4.10 t0

`t0 = 0`

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: 0

Definition at line 127 of file amimodel.m.

9.4.4.11 wtype

```
wtype = char.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: char.empty("")

Definition at line 138 of file amimodel.m.

9.4.4.12 nx

```
nx = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 149 of file amimodel.m.

9.4.4.13 nxtrue

```
nxtrue = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 160 of file amimodel.m.

9.4.4.14 ny

```
ny = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 171 of file amimodel.m.

9.4.4.15 nytrue

`nytrue = double.empty("")`

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 182 of file amimodel.m.

9.4.4.16 np

`np = double.empty("")`

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 193 of file amimodel.m.

9.4.4.17 nk

`nk = double.empty("")`

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 204 of file amimodel.m.

9.4.4.18 ng

`ng = double.empty("")`

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 215 of file amimodel.m.

9.4.4.19 nevent

```
nevent = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 226 of file amimodel.m.

9.4.4.20 nz

```
nz = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 237 of file amimodel.m.

9.4.4.21 nztrue

```
nztrue = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 248 of file amimodel.m.

9.4.4.22 id

```
id = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 259 of file amimodel.m.

9.4.4.23 ubw

```
ubw = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 270 of file amimodel.m.

9.4.4.24 lbw

```
lbw = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 281 of file amimodel.m.

9.4.4.25 nnz

```
nnz = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 292 of file amimodel.m.

9.4.4.26 sparseidx

```
sparseidx = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 303 of file amimodel.m.

9.4.4.27 rowvals

```
rowvals = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
Matlab documentation of property attributes.
Default: double.empty("")

Definition at line 314 of file amimodel.m.

9.4.4.28 colptrs

```
colptrs = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
Matlab documentation of property attributes.
Default: double.empty("")

Definition at line 325 of file amimodel.m.

9.4.4.29 sparseidxB

```
sparseidxB = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
Matlab documentation of property attributes.
Default: double.empty("")

Definition at line 336 of file amimodel.m.

9.4.4.30 rowvalsB

```
rowvalsB = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
Matlab documentation of property attributes.
Default: double.empty("")

Definition at line 347 of file amimodel.m.

9.4.4.31 colptrsB

```
colptrsB = double.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 358 of file amimodel.m.

9.4.4.32 funs

```
funs = cell.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: cell.empty("")

Definition at line 369 of file amimodel.m.

9.4.4.33 mfuns

```
mfuns = cell.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: cell.empty("")

Definition at line 380 of file amimodel.m.

9.4.4.34 coptim

```
coptim = "-O3"
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: "-O3"

Definition at line 391 of file amimodel.m.

9.4.4.35 param

```
param = "lin"
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
Matlab documentation of property attributes.
Default: "lin"

Definition at line 402 of file amimodel.m.

9.4.4.36 wrap_path

```
wrap_path = char.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
Matlab documentation of property attributes.
Default: char.empty("")

Definition at line 413 of file amimodel.m.

9.4.4.37 recompile

```
recompile = false
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
Matlab documentation of property attributes.
Default: false

Definition at line 424 of file amimodel.m.

9.4.4.38 cfun

```
cfun = struct.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
Matlab documentation of property attributes.
Default: struct.empty("")

Definition at line 435 of file amimodel.m.

9.4.4.39 o2flag

`o2flag = 0`

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: 0

Definition at line 447 of file amimodel.m.

9.4.4.40 z2event

`z2event = double.empty("")`

Default: double.empty("")

Definition at line 466 of file amimodel.m.

9.4.4.41 splineflag

`splineflag = false`

Default: false

Definition at line 474 of file amimodel.m.

9.4.4.42 minflag

`minflag = false`

Default: false

Definition at line 482 of file amimodel.m.

9.4.4.43 maxflag

`maxflag = false`

Default: false

Definition at line 490 of file amimodel.m.

9.4.4.44 nw

```
nw = 0
```

Default: 0

Definition at line 498 of file amimodel.m.

9.4.4.45 ndwdx

```
ndwdx = 0
```

Default: 0

Definition at line 507 of file amimodel.m.

9.4.4.46 ndwdp

```
ndwdp = 0
```

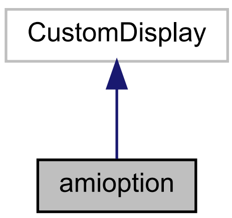
Default: 0

Definition at line 515 of file amimodel.m.

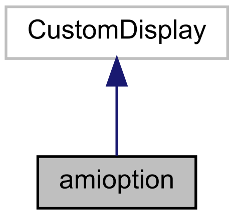
9.5 amioption Class Reference

AMIOPTION provides an option container to pass simulation parameters to the simulation routine.

Inheritance diagram for amioption:



Collaboration diagram for amioption:



Public Member Functions

- amioption (matlabtypesubstitute varargin)

    amioptions Construct a new amioptions object OPTS = amioption() creates a set of options with each option set to its default value.

Public Attributes

- matlabtypesubstitute atol = 1e-16

    absolute integration tolerace
- matlabtypesubstitute rtol = 1e-8

    relative integration tolerace
- matlabtypesubstitute maxsteps = 1e4

    maximum number of integration steps
- matlabtypesubstitute sens_ind = double.empty("")

    index of parameters for which the sensitivities are computed
- matlabtypesubstitute qpositivex = double.empty("")

    index of states for which positivity should be enforced
- matlabtypesubstitute pbar = double.empty("")

    scaling of error tolerances for sensitivity equations
- matlabtypesubstitute tstart = 0

    starting time of the simulation
- matlabtypesubstitute lmm = 2

    linear multistep method.
- matlabtypesubstitute iter = 2

    iteration method for linear multistep.
- matlabtypesubstitute linsol = 9

    linear solver
- matlabtypesubstitute stldet = true

    stability detection flag
- matlabtypesubstitute interpType = 1

    interpolation type
- matlabtypesubstitute lmmB = 2

    linear multistep method (backwards)
- matlabtypesubstitute iterB = 2

iteration method for linear multistep (backwards).
- matlabtypesubstitute ism = 1

  forward sensitivity mode
- matlabtypesubstitute sensi_meth = 1

  sensitivity method
- matlabtypesubstitute sensi = 0

  sensitivity order
- matlabtypesubstitute nmaxevent = 10

  number of reported events
- matlabtypesubstitute ordering = 0

  reordering of states
- matlabtypesubstitute ss = 0

  steady state sensitivity flag
- matlabtypesubstitute x0 = double.empty("")

  custom initial state
- matlabtypesubstitute sx0 = double.empty("")

  custom initial sensitivity
- matlabtypesubstitute newton_precon = 1

  newton solver: preconditioning method (0 = none, 1 = diagonal, 2 = incomplete LU)
- matlabtypesubstitute newton_maxsteps = 40

  newton solver: maximum newton steps
- matlabtypesubstitute newton_maxlinsteps = 100

  newton solver: maximum linear steps
- matlabtypesubstitute newton_preeq = false

  preequilibration of system via newton solver
- matlabtypesubstitute z2event = double.empty("")

  mapping of event ouputs to events
- matlabtypesubstitute pscale = ""

  parameter scaling Valid options are "log","log10" and "lin" for log, log10 or unscaled parameters p use "" for default as specified in the model (fallback: `lin`)
- matlabtypesubstitute id = double.empty("")

  flag for DAE variables

9.5.1 Detailed Description

Definition at line 17 of file amioption.m.

9.5.2 Constructor & Destructor Documentation

9.5.2.1 amioption()

```
amioption (
            matlabtypesubstitute varargin )
```

OPTS = amioption(PARAM, VAL, ...) creates a set of options with the named parameters altered with the specified values.

OPTS = amioption(OLDOPTS, PARAM, VAL, ...) creates a copy of OLDOPTS with the named parameters altered with the specified value

Note: to see the parameters, check the documentation page for

Parameters

varargin	input to construct amioption object, see function function description

Definition at line 274 of file amioption.m.

9.5.3 Member Data Documentation

9.5.3.1 atol

```
atol = 1e-16
```

Default: 1e-16

Definition at line 28 of file amioption.m.

9.5.3.2 rtol

```
rtol = 1e-8
```

Default: 1e-8

Definition at line 36 of file amioption.m.

9.5.3.3 maxsteps

```
maxsteps = 1e4
```

Default: 1e4

Definition at line 44 of file amioption.m.

9.5.3.4 sens_ind

```
sens_ind = double.empty("")
```

Default: double.empty("")

Definition at line 52 of file amioption.m.

9.5.3.5 qpositivex

```
qpositivex = double.empty("")
```

Default: double.empty("")

Definition at line 60 of file amioption.m.

9.5.3.6 pbar

```
pbar = double.empty("")
```

Default: double.empty("")

Definition at line 68 of file amioption.m.

9.5.3.7 tstart

```
tstart = 0
```

Default: 0

Definition at line 76 of file amioption.m.

9.5.3.8 lmm

```
lmm = 2
```

Default: 2

Definition at line 84 of file amioption.m.

9.5.3.9 iter

```
iter = 2
```

Default: 2

Definition at line 92 of file amioption.m.

9.5.3.10 linsol

```
linsol = 9
```

Default: 9

Definition at line 100 of file amioption.m.

9.5.3.11 stldet

```
stldet = true
```

Default: true

Definition at line 108 of file amioption.m.

9.5.3.12 interpType

```
interpType = 1
```

Default: 1

Definition at line 116 of file amioption.m.

9.5.3.13 lmmB

```
lmmB = 2
```

Default: 2

Definition at line 124 of file amioption.m.

9.5.3.14 iterB

```
iterB = 2
```

Default: 2

Definition at line 132 of file amioption.m.

9.5.3.15 ism

```
ism = 1
```

Default: 1

Definition at line 140 of file amioption.m.

9.5.3.16 sensi_meth

```
sensi_meth = 1
```

Default: 1

Note

This property has custom functionality when its value is changed.

Definition at line 148 of file amioption.m.

9.5.3.17 sensi

```
sensi = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 156 of file amioption.m.

9.5.3.18 nmaxevent

```
nmaxevent = 10
```

Default: 10

Definition at line 164 of file amioption.m.

9.5.3.19 ordering

```
ordering = 0
```

Default: 0

Definition at line 172 of file amioption.m.

9.5.3.20 ss

```
ss = 0
```

Default: 0

Definition at line 180 of file amioption.m.

9.5.3.21 x0

```
x0 = double.empty("")
```

Default: double.empty("")

Definition at line 188 of file amioption.m.

9.5.3.22 sx0

```
sx0 = double.empty("")
```

Default: double.empty("")

Definition at line 196 of file amioption.m.

9.5.3.23 newton_precon

```
newton_precon = 1
```

Default: 1

Note

This property has custom functionality when its value is changed.

Definition at line 204 of file amioption.m.

9.5.3.24 newton_maxsteps

```
newton_maxsteps = 40
```

Default: 40

Note

This property has custom functionality when its value is changed.

Definition at line 213 of file amioption.m.

9.5.3.25 newton_maxlinsteps

```
newton_maxlinsteps = 100
```

Default: 100

Note

This property has custom functionality when its value is changed.

Definition at line 221 of file amioption.m.

9.5.3.26 newton_preeq

```
newton_preeq = false
```

Default: false

Note

This property has custom functionality when its value is changed.

Definition at line 229 of file amioption.m.

9.5.3.27 z2event

```
z2event = double.empty("")
```

Default: double.empty("")

Definition at line 237 of file amioption.m.

9.5.3.28 pscale

```
pscale = ""
```

Default: ""

Note

This property has custom functionality when its value is changed.

Definition at line 245 of file amioption.m.

9.5.3.29 id

```
id = double.empty("")
```

Note

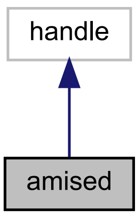
This property has the MATLAB attribute `Hidden` set to true.
`Matlab documentation of property attributes.`
Default: double.empty("")

Definition at line 260 of file amioption.m.

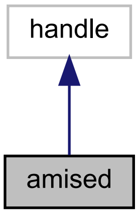
9.6 amised Class Reference

AMISED is a container for SED-ML objects.

Inheritance diagram for amised:



Collaboration diagram for amised:



Public Member Functions

- amised (matlabtypesubstitute sedname)
  amised reads in an SEDML document using the JAVA binding of of libSEDML

Public Attributes

- matlabtypesubstitute model = struct('"event',[ ],'sym',[ ]")
  amimodel from the specified model
- matlabtypesubstitute modelname = {""}
  cell array of model identifiers
- matlabtypesubstitute sedml = struct.empty("")
  stores the struct tree from the xml definition
- matlabtypesubstitute outputcount = "[ ]"
  count the number of outputs per model
- matlabtypesubstitute varidx = "[ ]"
  indexes for dataGenerators
- matlabtypesubstitute varsym = sym("[ ]")
  symbolic expressions for variables
- matlabtypesubstitute datasym = sym("[ ]")
  symbolic expressions for data

9.6.1 Detailed Description

Definition at line 17 of file amised.m.

9.6.2 Constructor & Destructor Documentation

9.6.2.1 amised()

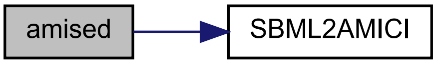
```
amised (
            matlabtypesubstitute sedname )
```

Parameters

sedname	name/path of the SEDML document

Definition at line 112 of file amised.m.

Here is the call graph for this function:



9.6.3 Member Data Documentation

9.6.3.1 model

```
model = struct("'event',[],'sym',[]")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: struct("'event',[ ],'sym',[ ]")

Definition at line 27 of file amised.m.

9.6.3.2 modelname

```
modelname = {""}
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: {""}

Definition at line 38 of file amised.m.

9.6.3.3 sedml

```
sedml = struct.empty("")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: struct.empty("")

Definition at line 49 of file amised.m.

9.6.3.4 outputcount

```
outputcount = "[]"
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: "[]"

Definition at line 60 of file amised.m.

9.6.3.5 varidx

```
varidx = "[]"
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: "[]"

Definition at line 71 of file amised.m.

9.6.3.6 varsym

```
varsym = sym("[]")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: sym("[]")

Definition at line 82 of file amised.m.

9.6.3.7 datasym

```
datasym = sym("[]")
```

Note

This property has non-standard access specifiers: `SetAccess = Private, GetAccess = Public`
`Matlab documentation of property attributes.`
Default: sym("[]")

Definition at line 93 of file amised.m.

9.7 BackwardProblem Class Reference

class to solve backwards problems.

`#include <backwardproblem.h>`

Static Public Member Functions

- static int workBackwardProblem (UserData ∗udata, TempData ∗tdata, ReturnData ∗rdata, Model ∗model)
- static int handleEventB (int iroot, TempData ∗tdata, Model ∗model)
- static int handleDataPointB (int it, ReturnData ∗rdata, TempData ∗tdata, Solver ∗solver, Model ∗model)
- static int updateHeavisideB (int iroot, TempData ∗tdata, int ne)
- static realtype getTnext (realtype ∗troot, int iroot, realtype ∗tdata, int it, Model ∗model)

9.7.1 Detailed Description

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

Definition at line 19 of file backwardproblem.h.

9.7.2 Member Function Documentation

9.7.2.1 workBackwardProblem()

```
int workBackwardProblem (
            UserData * udata,
            TempData * tdata,
            ReturnData * rdata,
            Model * model )  [static]
```

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

Parameters

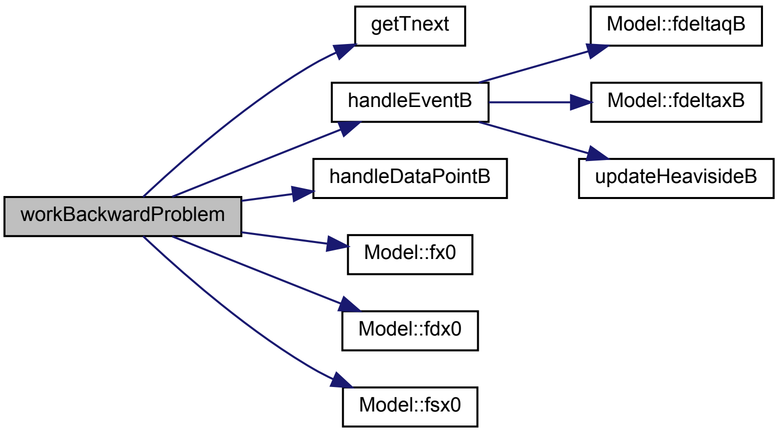
in	*udata*	pointer to the user data struct **Type**: UserData
in	*tdata*	pointer to the temporary data struct **Type**: TempData
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*model*	pointer to model specification object **Type**: Model

Returns

int status flag

Definition at line 10 of file backwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

9.7.2.2 handleEventB()

```
int handleEventB (
            int iroot,
            TempData * tdata,
            Model * model )  [static]
```

handleEventB executes everything necessary for the handling of events for the backward problem

Parameters

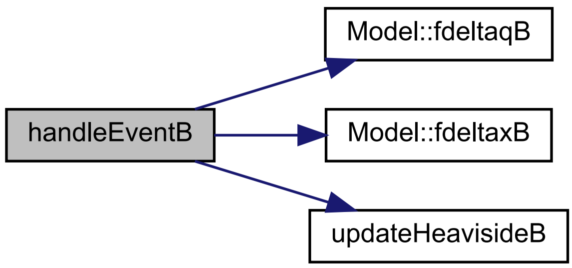
out	*iroot*	index of event **Type**: int
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*model*	pointer to model specification object **Type**: Model

Returns

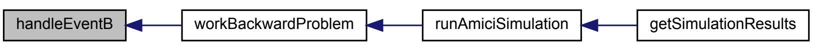
status flag indicating success of execution
Type: int

Definition at line 174 of file backwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.7.2.3 handleDataPointB()

```
int handleDataPointB (
            int it,
            ReturnData * rdata,
            TempData * tdata,
            Solver * solver,
            Model * model )  [static]
```

handleDataPoint executes everything necessary for the handling of data points for the backward problems

Parameters

in	*it*	index of data point **Type**: int
out	*rdata*	pointer to the return data struct **Type**: ReturnData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*solver*	pointer to solver object **Type**: Solver
in	*model*	pointer to model specification object **Type**: Model

Returns

status flag indicating success of execution
Type: int

Definition at line 246 of file backwardproblem.cpp.

Here is the caller graph for this function:

9.7.2.4 updateHeavisideB()

```
int updateHeavisideB (
            int iroot,
            TempData * tdata,
            int ne )  [static]
```

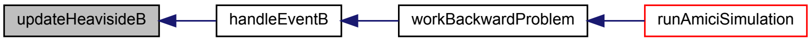
updateHeavisideB updates the heaviside variables h on event occurences for the backward problem

Parameters

in	*iroot*	discontinuity occurance index **Type**: int
out	*tdata*	pointer to the temporary data struct **Type**: TempData

Definition at line 277 of file backwardproblem.cpp.

Here is the caller graph for this function:



9.7.2.5 getTnext()

```
realtype getTnext (
            realtype * troot,
            int iroot,
            realtype * tdata,
            int it,
            Model * model ) [static]
```

getTnext computes the next timepoint to integrate to. This is the maximum of tdata and troot but also takes into account if it<0 or iroot<0 where these expressions do not necessarily make sense

Parameters

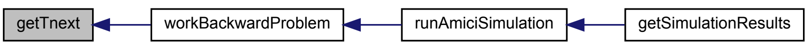
in	*troot*	timepoint of next event **Type**: realtype
in	*iroot*	index of next event **Type**: int
in	*tdata*	timepoint of next data point **Type**: realtype
in	*it*	index of next data point **Type**: int
in	*model*	pointer to model specification object **Type**: Model

Returns

tnext next timepoint
Type: realtype

Definition at line 301 of file backwardproblem.cpp.

Here is the caller graph for this function:



9.8 ExpData Class Reference

struct that carries all information about experimental data

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

Public Member Functions

- ExpData ()
  Default constructor.
- ExpData (const UserData *udata, Model *model)
- void setDefaults ()

Public Attributes

- double * my
- double * sigmay
- double * mz
- double * mrz
- double * sigmaz

9.8.1 Detailed Description

Definition at line 8 of file edata.h.

9.8.2 Constructor & Destructor Documentation

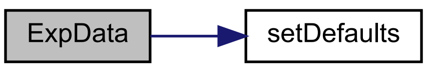
9.8.2.1 ExpData()

```
ExpData (
            const UserData * udata,
            Model * model )
```

initialization with UserData and model

Definition at line 9 of file edata.cpp.

Here is the call graph for this function:



9.8.3 Member Function Documentation

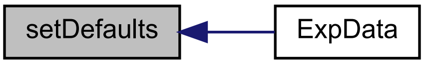
9.8.3.1 setDefaults()

```
void setDefaults ( )
```

initialization with default values

Definition at line 20 of file edata.cpp.

Here is the caller graph for this function:



9.8.4 Member Data Documentation

9.8.4.1 my

```
double* my
```

observed data

Definition at line 23 of file edata.h.

9.8.4.2 sigmay

```
double* sigmay
```

standard deviation of observed data

Definition at line 25 of file edata.h.

9.8.4.3 mz

```
double* mz
```

observed events

Definition at line 28 of file edata.h.

9.8.4.4 mrz

```
double* mrz
```

observed roots

Definition at line 30 of file edata.h.

9.8.4.5 sigmaz

```
double* sigmaz
```

standard deviation of observed events/roots

Definition at line 32 of file edata.h.

9.9 ForwardProblem Class Reference

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

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

Static Public Member Functions

- static int workForwardProblem (UserData *udata, TempData *tdata, ReturnData *rdata, const ExpData *edata, Model *model)
- static int handleEvent (realtype *tlastroot, UserData *udata, ReturnData *rdata, const ExpData *edata, TempData *tdata, int seflag, Solver *solver, Model *model)
- static int storeJacobianAndDerivativeInReturnData (TempData *tdata, ReturnData *rdata, Model *model)
- static int getEventOutput (UserData *udata, ReturnData *rdata, const ExpData *edata, TempData *tdata, Model *model)
- static int prepEventSensis (int ie, ReturnData *rdata, const ExpData *edata, TempData *tdata, Model *model)
- static int getEventSensisFSA (int ie, ReturnData *rdata, const ExpData *edata, TempData *tdata, Model *model)
- static int handleDataPoint (int it, UserData *udata, ReturnData *rdata, const ExpData *edata, TempData *tdata, Solver *solver, Model *model)
- static int getDataOutput (int it, UserData *udata, ReturnData *rdata, const ExpData *edata, TempData *tdata, Solver *solver, Model *model)
- static int prepDataSensis (int it, ReturnData *rdata, const ExpData *edata, TempData *tdata, Model *model)
- static int getDataSensisFSA (int it, UserData *udata, ReturnData *rdata, const ExpData *edata, TempData *tdata, Solver *solver, Model *model)
- static int applyEventBolus (TempData *tdata, Model *model)
- static int applyEventSensiBolusFSA (TempData *tdata, Model *model)
- static int updateHeaviside (TempData *tdata, int ne)

9.9.1 Detailed Description

Definition at line 18 of file forwardproblem.h.

9.9.2 Member Function Documentation

9.9.2.1 workForwardProblem()

```
int workForwardProblem (
            UserData * udata,
            TempData * tdata,
            ReturnData * rdata,
            const ExpData * edata,
            Model * model ) [static]
```

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

Parameters

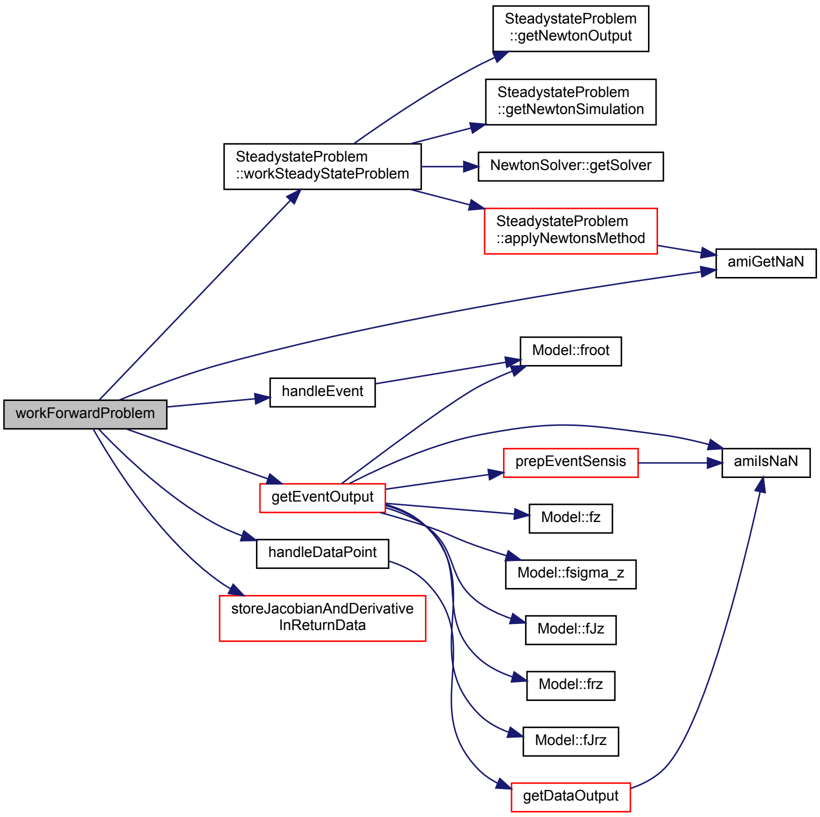
in	*udata*	pointer to the user data struct **Type**: UserData
in	*tdata*	pointer to the temporary data struct **Type**: TempData
out	*rdata*	pointer to the return data struct **Type**: ReturnData
out	*edata*	pointer to the experimental data struct **Type**: ExpData
in	*model*	pointer to model specification object **Type**: Model

Returns

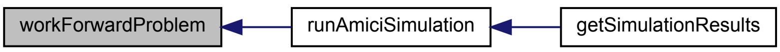
int status flag indicating success of execution
Type: int

Definition at line 11 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.2 handleEvent()

```
int handleEvent (
            realtype * tlastroot,
            UserData * udata,
            ReturnData * rdata,
            const ExpData * edata,
            TempData * tdata,
            int seflag,
            Solver * solver,
            Model * model ) [static]
```

handleEvent executes everything necessary for the handling of events

Parameters

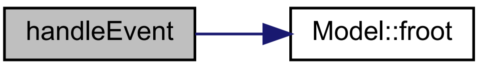
out	*tlastroot*	pointer to the timepoint of the last event **Type**: ∗realtype
in	*udata*	pointer to the user data struct **Type**: UserData
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*edata*	pointer to the experimental data struct **Type**: ExpData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*seflag*	flag indicating whether this is a secondary event **Type**: int
in	*solver*	pointer to solver object **Type**: Solver
in	*model*	pointer to model specification object **Type**: Model

Returns

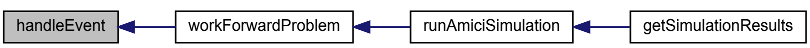
status flag indicating success of execution
Type: int

Definition at line 123 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.3 storeJacobianAndDerivativeInReturnData()

```
int storeJacobianAndDerivativeInReturnData (
            TempData * tdata,
            ReturnData * rdata,
            Model * model )  [static]
```

evalues the Jacobian and differential equation right hand side, stores it in tdata and and copies it to rdata

Parameters

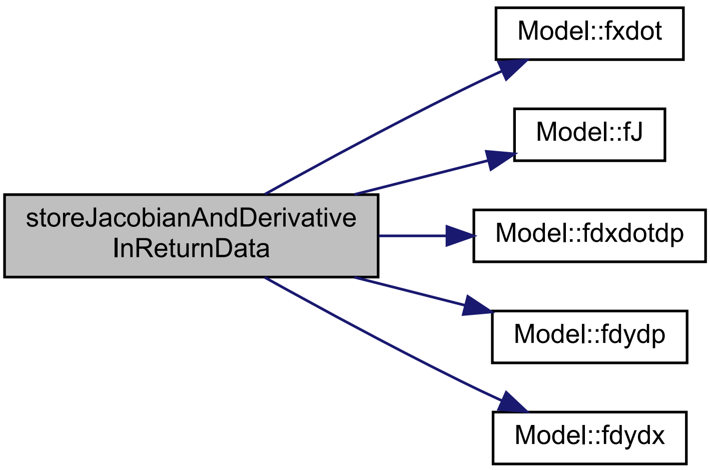
out	*tdata*	pointer to the temporary data struct **Type**: TempData
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*model*	pointer to model specification object **Type**: Model

Returns

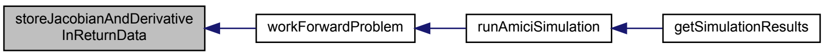
void

Definition at line 321 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.4 getEventOutput()

```
int getEventOutput (
            UserData * udata,
            ReturnData * rdata,
            const ExpData * edata,
            TempData * tdata,
            Model * model ) [static]
```

getEventOutput extracts output information for events

Parameters

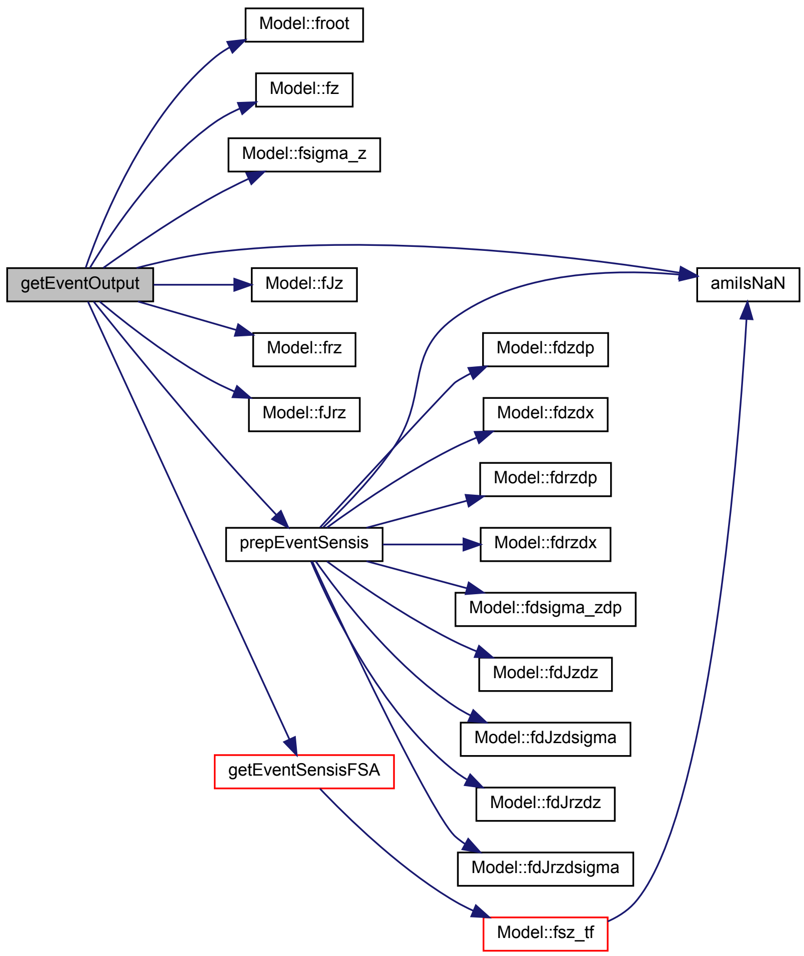
in	*udata*	pointer to the user data struct **Type**: UserData
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*edata*	pointer to the experimental data struct **Type**: ExpData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*model*	pointer to model specification object **Type**: Model

Returns

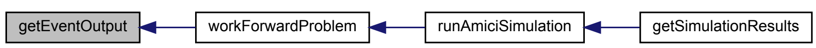
status flag indicating success of execution
Type: int

Definition at line 396 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.5 prepEventSensis()

```
int prepEventSensis (
            int ie,
            ReturnData * rdata,
            const ExpData * edata,
```

```
TempData * tdata,
Model * model ) [static]
```

prepEventSensis preprocesses the provided experimental data to compute event sensitivities via adjoint or forward methods later on

Parameters

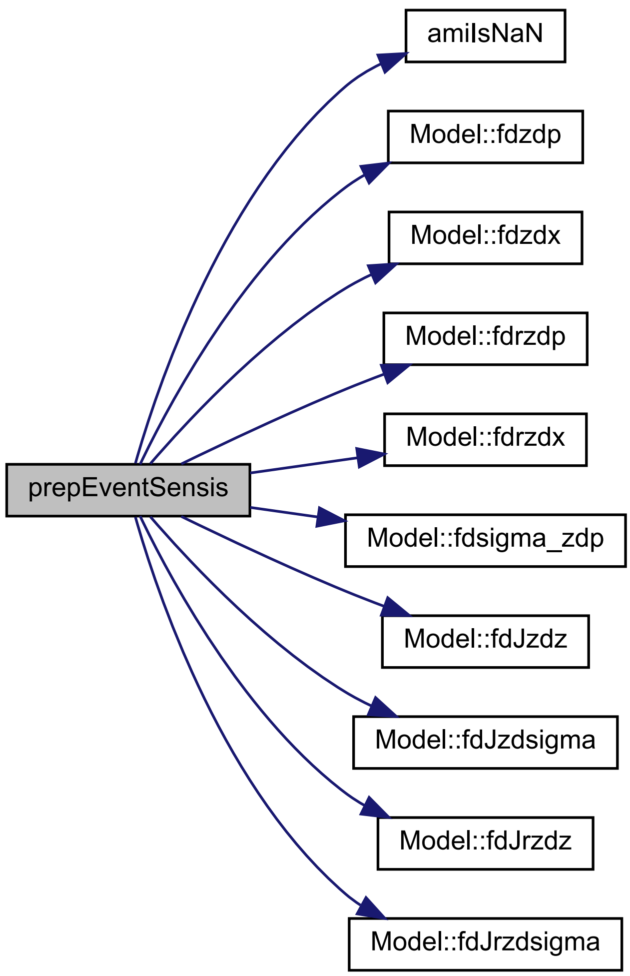
in	*ie*	index of current event **Type**: int
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*edata*	pointer to the experimental data struct **Type**: ExpData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*model*	pointer to model specification object **Type**: Model

Returns

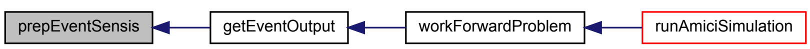
status flag indicating success of execution
Type: int

Definition at line 495 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.6 getEventSensisFSA()

```
int getEventSensisFSA (
            int ie,
```

```
ReturnData * rdata,
const ExpData * edata,
TempData * tdata,
Model * model ) [static]
```

getEventSensisFSA extracts event information for forward sensitivity analysis

Parameters

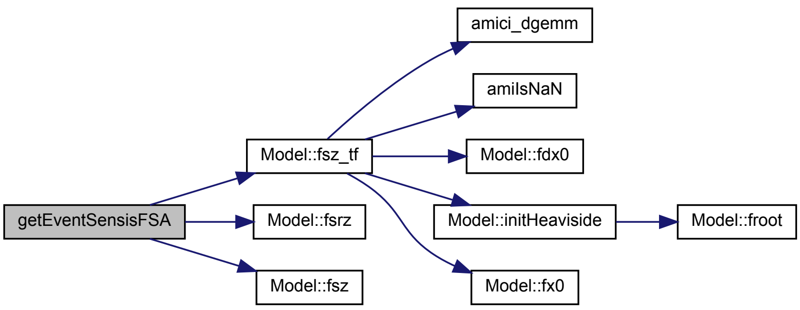
in	*ie*	index of event type **Type**: int
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*edata*	pointer to the experimental data struct **Type**: ExpData
in	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*model*	pointer to model specification object **Type**: Model

Returns

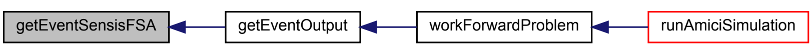
status flag indicating success of execution
Type: int

Definition at line 608 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.7 handleDataPoint()

```
int handleDataPoint (
            int it,
            UserData * udata,
            ReturnData * rdata,
            const ExpData * edata,
            TempData * tdata,
            Solver * solver,
            Model * model ) [static]
```

handleDataPoint executes everything necessary for the handling of data points

Parameters

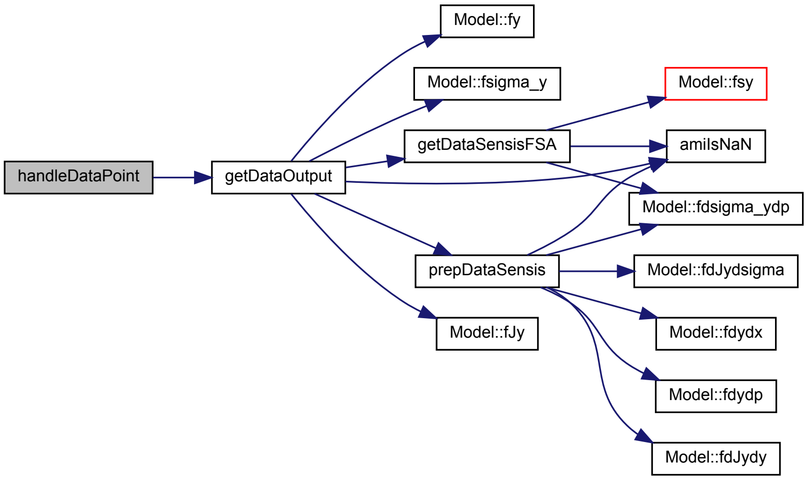
in	*it*	index of data point **Type**: int
in	*udata*	pointer to the user data struct **Type**: UserData
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*edata*	pointer to the experimental data struct **Type**: ExpData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*solver*	pointer to solver object **Type**: Solver
in	*model*	pointer to model specification object **Type**: Model

Returns

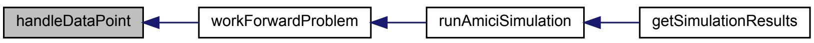
status flag indicating success of execution
Type: int

Definition at line 651 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.8 getDataOutput()

```
int getDataOutput (
            int it,
            UserData * udata,
            ReturnData * rdata,
            const ExpData * edata,
            TempData * tdata,
            Solver * solver,
            Model * model ) [static]
```

getDataOutput extracts output information for data-points

Parameters

in	*it*	index of current timepoint **Type**: int
in	*udata*	pointer to the user data struct **Type**: UserData
out	*rdata*	pointer to the return data struct **Type**: ReturnData

Parameters

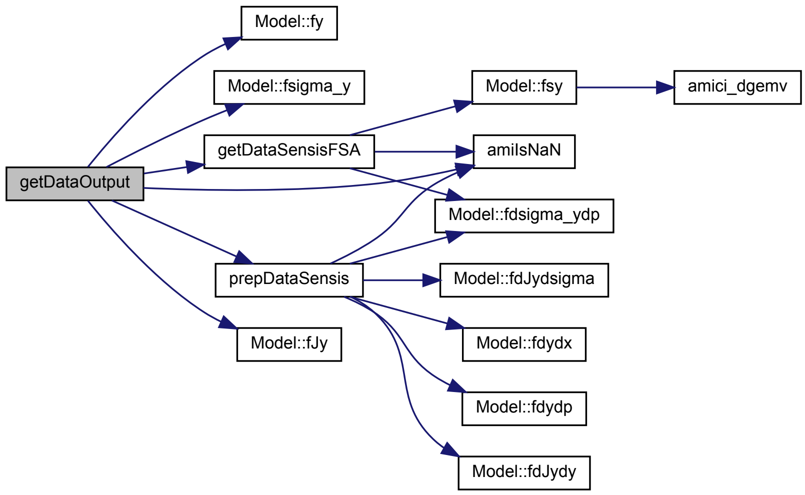
in	*edata*	pointer to the experimental data struct **Type**: ExpData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*solver*	pointer to solver object **Type**: Solver
in	*model*	pointer to model specification object **Type**: Model

Returns

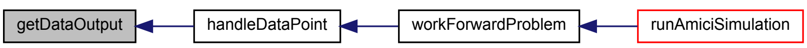
status flag indicating success of execution
Type: int

Definition at line 690 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.9 prepDataSensis()

```
int prepDataSensis (
            int it,
            ReturnData * rdata,
            const ExpData * edata,
            TempData * tdata,
            Model * model )  [static]
```

prepDataSensis preprocesses the provided experimental data to compute sensitivities via adjoint or forward methods later on

Parameters

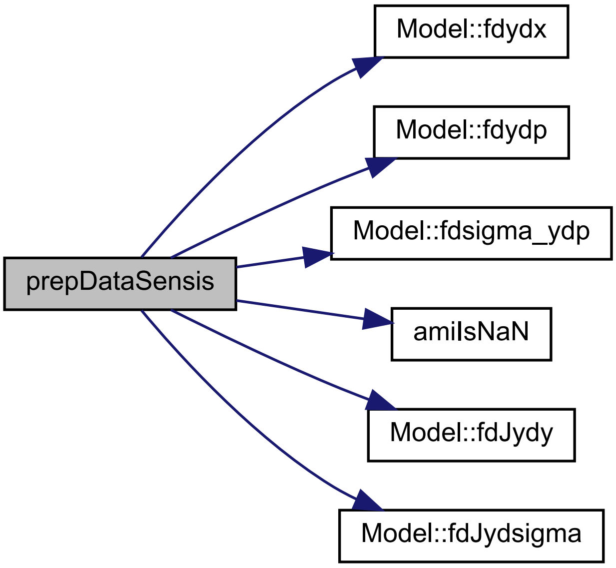
in	*it*	index of current timepoint **Type**: int
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*edata*	pointer to the experimental data struct **Type**: ExpData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*model*	pointer to model specification object **Type**: Model

Returns

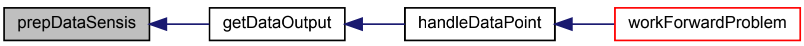
status flag indicating success of execution
Type: int

Definition at line 752 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.10 getDataSensisFSA()

```
int getDataSensisFSA (
            int it,
            UserData * udata,
            ReturnData * rdata,
            const ExpData * edata,
            TempData * tdata,
            Solver * solver,
            Model * model )  [static]
```

getDataSensisFSA extracts data information for forward sensitivity analysis

Parameters

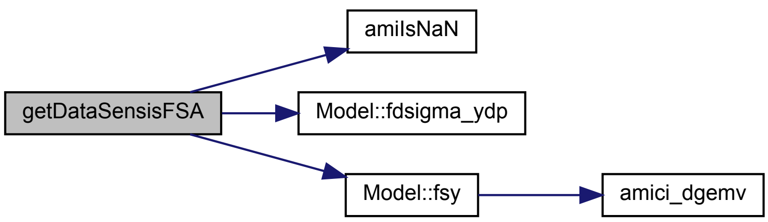
out	*status*	flag indicating success of execution **Type**: int
in	*it*	index of current timepoint **Type**: int
in	*udata*	pointer to the user data struct **Type**: UserData
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*edata*	pointer to the experimental data struct **Type**: ExpData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*solver*	pointer to solver object **Type**: Solver
in	*model*	pointer to model specification object **Type**: Model

Returns

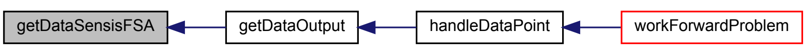
void

Definition at line 833 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.9.2.11 applyEventBolus()

```
int applyEventBolus (
            TempData * tdata,
            Model * model )  [static]
```

applyEventBolus applies the event bolus to the current state

Parameters

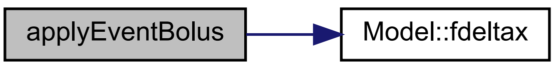
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*model*	pointer to model specification object **Type**: Model

Returns

status flag indicating success of execution
Type: int

Definition at line 906 of file forwardproblem.cpp.

Here is the call graph for this function:



9.9.2.12 applyEventSensiBolusFSA()

```
int applyEventSensiBolusFSA (
            TempData * tdata,
            Model * model ) [static]
```

applyEventSensiBolusFSA applies the event bolus to the current sensitivities

Parameters

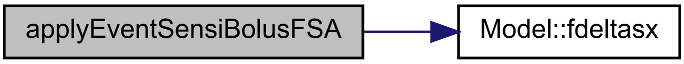
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*model*	pointer to model specification object **Type**: Model

Returns

status flag indicating success of execution
Type: int

Definition at line 942 of file forwardproblem.cpp.

Here is the call graph for this function:



9.9.2.13 updateHeaviside()

```
int updateHeaviside (
            TempData * tdata,
            int ne )  [static]
```

updateHeaviside updates the heaviside variables h on event occurences

Parameters

Definition at line 980 of file forwardproblem.cpp.

9.10 Model Class Reference

The Model class represents an AMICI ODE model. The model does not contain any data, its state should never change.

```
#include <amici_model.h>
```

Public Member Functions

- **Model** (int np, int nx, int nxtrue, int nk, int ny, int nytrue, int nz, int nztrue, int ne, int nJ, int nw, int ndwdx, int ndwdp, int nnz, int ubw, int lbw, AMICI_o2mode o2mode)
- virtual Solver ∗ **getSolver** ()
- virtual int fx0 (N_Vector x0, void ∗user_data)
- virtual int fdx0 (N_Vector x0, N_Vector dx0, void ∗user_data)
- virtual int fsx0 (N_Vector ∗sx0, N_Vector x, N_Vector dx, void ∗user_data)
- virtual int fsdx0 (N_Vector ∗sdx0, N_Vector x, N_Vector dx, void ∗user_data)
- virtual int fJ (long int N, realtype t, realtype cj, N_Vector x, N_Vector dx, N_Vector xdot, DlsMat J, void ∗user_data, N_Vector tmp1, N_Vector tmp2, N_Vector tmp3)
- virtual int fJB (long int NeqBdot, realtype t, N_Vector x, N_Vector xB, N_Vector xBdot, DlsMat JB, void ∗user_data, N_Vector tmp1B, N_Vector tmp2B, N_Vector tmp3B)
- virtual int fJDiag (realtype t, N_Vector JDiag, N_Vector x, void ∗user_data)
- virtual int fJv (N_Vector v, N_Vector Jv, realtype t, N_Vector x, N_Vector xdot, void ∗user_data, N_Vector tmp)
- virtual int froot (realtype t, N_Vector x, N_Vector dx, realtype ∗root, void ∗user_data)

- virtual int frz (realtype t, int ie, N_Vector x, TempData *tdata, ReturnData *rdata)
- virtual int fsrz (realtype t, int ie, N_Vector x, N_Vector *sx, TempData *tdata, ReturnData *rdata)
- virtual int fstau (realtype t, int ie, N_Vector x, N_Vector *sx, TempData *tdata)
- virtual int fy (realtype t, int it, N_Vector x, void *user_data, ReturnData *rdata)
- virtual int fdydp (realtype t, int it, N_Vector x, TempData *tdata)
- virtual int fdydx (realtype t, int it, N_Vector x, TempData *tdata)
- virtual int fz (realtype t, int ie, N_Vector x, TempData *tdata, ReturnData *rdata)
- virtual int fsz (realtype t, int ie, N_Vector x, N_Vector *sx, TempData *tdata, ReturnData *rdata)
- virtual int fdzdp (realtype t, int ie, N_Vector x, TempData *tdata)
- virtual int fdzdx (realtype t, int ie, N_Vector x, TempData *tdata)
- virtual int fdrzdp (realtype t, int ie, N_Vector x, TempData *tdata)
- virtual int fdrzdx (realtype t, int ie, N_Vector x, TempData *tdata)
- virtual int fxdot (realtype t, N_Vector x, N_Vector dx, N_Vector xdot, void *user_data)
- virtual int fxBdot (realtype t, N_Vector x, N_Vector xB, N_Vector xBdot, void *user_data)
- virtual int fqBdot (realtype t, N_Vector x, N_Vector xB, N_Vector qBdot, void *user_data)
- virtual int fdxdotdp (realtype t, N_Vector x, N_Vector dx, void *user_data)
- virtual int fdeltax (realtype t, int ie, N_Vector x, N_Vector xdot, N_Vector xdot_old, TempData *tdata)
- virtual int fdeltasx (realtype t, int ie, N_Vector x, N_Vector xdot, N_Vector xdot_old, N_Vector *sx, TempData *tdata)
- virtual int fdeltaxB (realtype t, int ie, N_Vector x, N_Vector xB, N_Vector xdot, N_Vector xdot_old, TempData *tdata)
- virtual int fdeltaqB (realtype t, int ie, N_Vector x, N_Vector xB, N_Vector qBdot, N_Vector xdot, N_Vector xdot_old, TempData *tdata)
- virtual int fsigma_y (realtype t, TempData *tdata)
- virtual int fdsigma_ydp (realtype t, TempData *tdata)
- virtual int fsigma_z (realtype t, int ie, TempData *tdata)
- virtual int fdsigma_zdp (realtype t, int ie, TempData *tdata)
- virtual int fJy (realtype t, int it, N_Vector x, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- virtual int fJz (realtype t, int ie, N_Vector x, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- virtual int fJrz (realtype t, int ie, N_Vector x, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- virtual int fdJydy (realtype t, int it, N_Vector x, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- virtual int fdJydsigma (realtype t, int it, N_Vector x, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- virtual int fdJzdz (realtype t, int ie, N_Vector x, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- virtual int fdJzdsigma (realtype t, int ie, N_Vector x, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- virtual int fdJrzdz (realtype t, int ie, N_Vector x, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- virtual int fdJrzdsigma (realtype t, int ie, N_Vector x, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- virtual int fsxdot (int Ns, realtype t, N_Vector x, N_Vector xdot, int ip, N_Vector sx, N_Vector sxdot, void *user_data, N_Vector tmp1, N_Vector tmp2)
- virtual int fJSparse (realtype t, N_Vector x, N_Vector xdot, SlsMat J, void *user_data, N_Vector tmp1, N_Vector tmp2, N_Vector tmp3)
- virtual int fJBand (long int N, long int mupper, long int mlower, realtype t, N_Vector x, N_Vector xdot, DlsMat J, void *user_data, N_Vector tmp1, N_Vector tmp2, N_Vector tmp3)
- virtual int fJBandB (long int NeqBdot, long int mupper, long int mlower, realtype t, N_Vector x, N_Vector xB, N_Vector xBdot, DlsMat JB, void *user_data, N_Vector tmp1B, N_Vector tmp2B, N_Vector tmp3B)
- virtual int fJvB (N_Vector vB, N_Vector JvB, realtype t, N_Vector x, N_Vector xB, N_Vector xBdot, void *user_data, N_Vector tmpB)
- virtual int fJSparseB (realtype t, N_Vector x, N_Vector xB, N_Vector xBdot, SlsMat JB, void *user_data, N_Vector tmp1B, N_Vector tmp2B, N_Vector tmp3B)
- int fsy (int it, TempData *tdata, ReturnData *rdata)
- int fsz_tf (int ie, TempData *tdata, ReturnData *rdata)
- int **fsJy** (int it, TempData *tdata, ReturnData *rdata)
- int **fdJydp** (int it, TempData *tdata, const ExpData *edata, ReturnData *rdata)

- int **fdJydx** (int it, TempData *tdata, const ExpData *edata)
- int **fsJz** (int ie, TempData *tdata, const ReturnData *rdata)
- int **fdJzdp** (int ie, TempData *tdata, const ExpData *edata, ReturnData *rdata)
- int **fdJzdx** (int ie, TempData *tdata, const ExpData *edata)
- int **initialize** (UserData *udata, TempData *tdata)
- int **initializeStates** (double *x0data, TempData *tdata)
- int initHeaviside (TempData *tdata)

Public Attributes

- const int np
- const int nk
- const int nx
- const int nxtrue
- 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 AMICI_o2mode o2mode
- int * z2event = nullptr
- realtype * idlist = nullptr

9.10.1 Detailed Description

Definition at line 16 of file amici_model.h.

9.10.2 Member Function Documentation

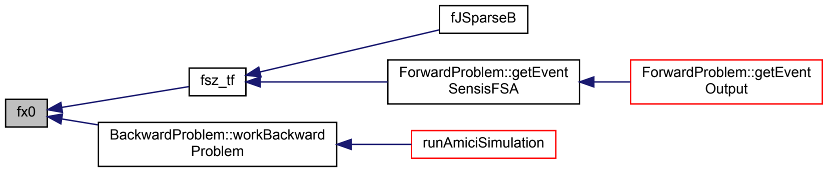
9.10.2.1 fx0()

```
virtual int fx0 (
            N_Vector x0,
            void * user_data ) [virtual]
```

Initial states

Definition at line 33 of file amici_model.h.

Here is the caller graph for this function:



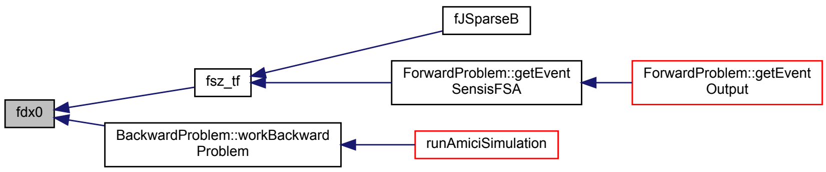
9.10.2.2 fdx0()

```
virtual int fdx0 (
            N_Vector x0,
            N_Vector dx0,
            void * user_data )  [virtual]
```

Initial value for time derivative of states

Definition at line 36 of file amici_model.h.

Here is the caller graph for this function:



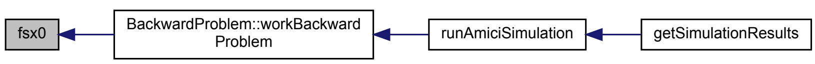
9.10.2.3 fsx0()

```
virtual int fsx0 (
            N_Vector * sx0,
            N_Vector x,
            N_Vector dx,
            void * user_data )  [virtual]
```

Initial value for time derivative of states

Definition at line 41 of file amici_model.h.

Here is the caller graph for this function:



9.10.2.4 fsdx0()

```
virtual int fsdx0 (
            N_Vector * sdx0,
            N_Vector x,
            N_Vector dx,
            void * user_data ) [virtual]
```

Sensitivity of initial states x0

Definition at line 44 of file amici_model.h.

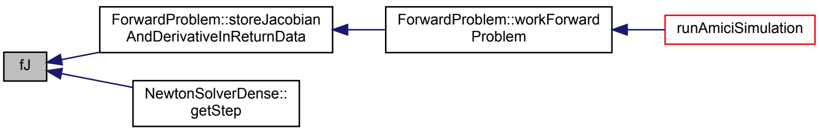
9.10.2.5 fJ()

```
virtual int fJ (
            long int N,
            realtype t,
            realtype cj,
            N_Vector x,
            N_Vector dx,
            N_Vector xdot,
            DlsMat J,
            void * user_data,
            N_Vector tmp1,
            N_Vector tmp2,
            N_Vector tmp3 ) [virtual]
```

Jacobian of xdot with respect to states x

Definition at line 47 of file amici_model.h.

Here is the caller graph for this function:



9.10.2.6 fJB()

```
virtual int fJB (
            long int NeqBdot,
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector xBdot,
            DlsMat JB,
            void * user_data,
            N_Vector tmp1B,
            N_Vector tmp2B,
            N_Vector tmp3B ) [virtual]
```

Jacobian of xBdot with respect to adjoint state xB

Definition at line 50 of file amici_model.h.

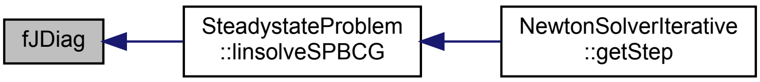
9.10.2.7 fJDiag()

```
virtual int fJDiag (
            realtype t,
            N_Vector JDiag,
            N_Vector x,
            void * user_data ) [virtual]
```

diagonalized Jacobian (for preconditioning)

Definition at line 53 of file amici_model.h.

Here is the caller graph for this function:



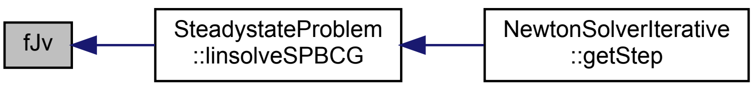
9.10.2.8 fJv()

```
virtual int fJv (
            N_Vector v,
            N_Vector Jv,
            realtype t,
            N_Vector x,
            N_Vector xdot,
            void * user_data,
            N_Vector tmp ) [virtual]
```

Matrix vector product of J with a vector v (for iterative solvers)

Definition at line 56 of file amici_model.h.

Here is the caller graph for this function:



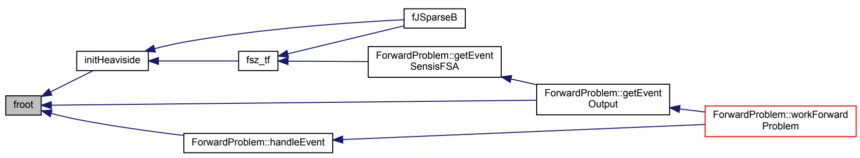
9.10.2.9 froot()

```
virtual int froot (
            realtype t,
            N_Vector x,
            N_Vector dx,
            realtype * root,
            void * user_data )  [virtual]
```

Event trigger function for events

Definition at line 59 of file amici_model.h.

Here is the caller graph for this function:



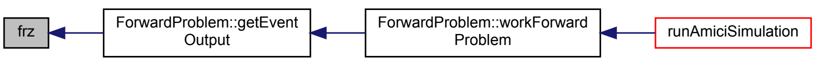
9.10.2.10 frz()

```
virtual int frz (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata,
            ReturnData * rdata )  [virtual]
```

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

Definition at line 62 of file amici_model.h.

Here is the caller graph for this function:



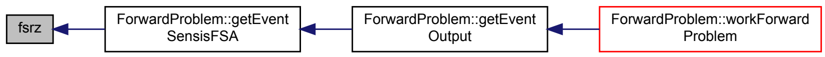
9.10.2.11 fsrz()

```
virtual int fsrz (
            realtype t,
            int ie,
            N_Vector x,
            N_Vector * sx,
            TempData * tdata,
            ReturnData * rdata ) [virtual]
```

Sensitivity of rz, total derivative

Definition at line 65 of file amici_model.h.

Here is the caller graph for this function:



9.10.2.12 fstau()

```
virtual int fstau (
            realtype t,
            int ie,
            N_Vector x,
            N_Vector * sx,
            TempData * tdata ) [virtual]
```

Sensitivity of event timepoint, total derivative

Definition at line 68 of file amici_model.h.

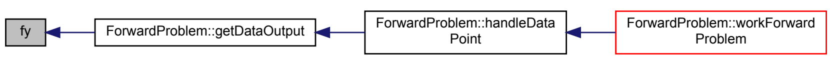
9.10.2.13 fy()

```
virtual int fy (
            realtype t,
            int it,
            N_Vector x,
            void * user_data,
            ReturnData * rdata ) [virtual]
```

Observables / measurements

Definition at line 71 of file amici_model.h.

Here is the caller graph for this function:



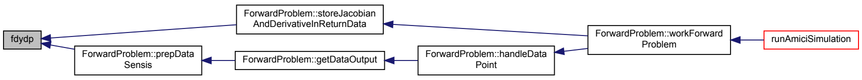
9.10.2.14 fdydp()

```
virtual int fdydp (
            realtype t,
            int it,
            N_Vector x,
            TempData * tdata )  [virtual]
```

Sensitivity of observables y w.r.t. model parameters p

Definition at line 74 of file amici_model.h.

Here is the caller graph for this function:



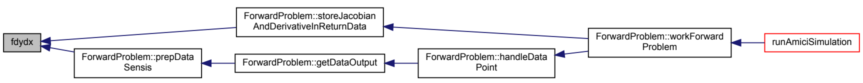
9.10.2.15 fdydx()

```
virtual int fdydx (
            realtype t,
            int it,
            N_Vector x,
            TempData * tdata )  [virtual]
```

Sensitivity of observables y w.r.t. state variables x

Definition at line 77 of file amici_model.h.

Here is the caller graph for this function:



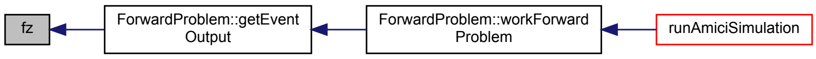
9.10.2.16 fz()

```
virtual int fz (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata,
            ReturnData * rdata )  [virtual]
```

Event-resolved measurements

Definition at line 80 of file amici_model.h.

Here is the caller graph for this function:



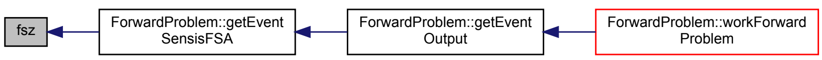
9.10.2.17 fsz()

```
virtual int fsz (
            realtype t,
            int ie,
            N_Vector x,
            N_Vector * sx,
            TempData * tdata,
            ReturnData * rdata )  [virtual]
```

Sensitivity of z, total derivative

Definition at line 83 of file amici_model.h.

Here is the caller graph for this function:



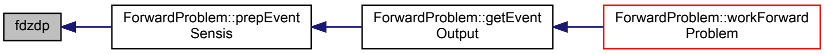
9.10.2.18 fdzdp()

```
virtual int fdzdp (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata ) [virtual]
```

Sensitivity of event-resolved measurements z w.r.t. to model parameters p

Definition at line 86 of file amici_model.h.

Here is the caller graph for this function:



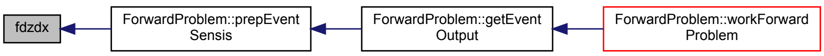
9.10.2.19 fdzdx()

```
virtual int fdzdx (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata ) [virtual]
```

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

Definition at line 89 of file amici_model.h.

Here is the caller graph for this function:



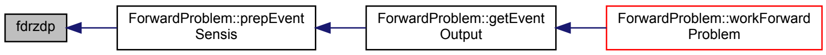
9.10.2.20 fdrzdp()

```
virtual int fdrzdp (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata )  [virtual]
```

Sensitivity of event-resolved measurements rz w.r.t. to model parameters p

Definition at line 92 of file amici_model.h.

Here is the caller graph for this function:



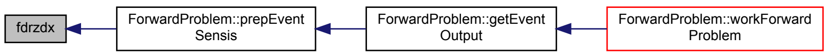
9.10.2.21 fdrzdx()

```
virtual int fdrzdx (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata )  [virtual]
```

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

Definition at line 95 of file amici_model.h.

Here is the caller graph for this function:



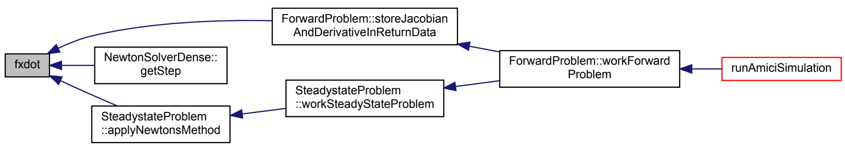
9.10.2.22 fxdot()

```
virtual int fxdot (
            realtype t,
            N_Vector x,
            N_Vector dx,
            N_Vector xdot,
            void * user_data ) [virtual]
```

Right hand side of differential equation for states x

Definition at line 98 of file amici_model.h.

Here is the caller graph for this function:



9.10.2.23 fxBdot()

```
virtual int fxBdot (
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector xBdot,
            void * user_data ) [virtual]
```

Right hand side of differential equation for adjoint state xB

Definition at line 101 of file amici_model.h.

9.10.2.24 fqBdot()

```
virtual int fqBdot (
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector qBdot,
            void * user_data ) [virtual]
```

Right hand side of integral equation for quadrature states qB

Definition at line 104 of file amici_model.h.

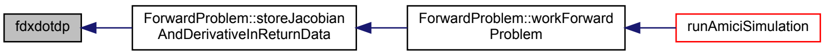
9.10.2.25 fdxdotdp()

```
virtual int fdxdotdp (
            realtype t,
            N_Vector x,
            N_Vector dx,
            void * user_data ) [virtual]
```

Sensitivity of dx/dt w.r.t. model parameters p

Definition at line 107 of file amici_model.h.

Here is the caller graph for this function:



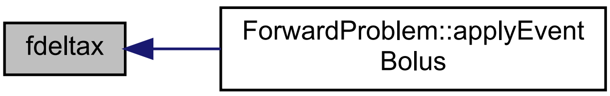
9.10.2.26 fdeltax()

```
virtual int fdeltax (
            realtype t,
            int ie,
            N_Vector x,
            N_Vector xdot,
            N_Vector xdot_old,
            TempData * tdata ) [virtual]
```

State update functions for events

Definition at line 110 of file amici_model.h.

Here is the caller graph for this function:



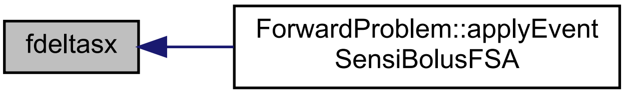
9.10.2.27 fdeltasx()

```
virtual int fdeltasx (
            realtype t,
            int ie,
            N_Vector x,
            N_Vector xdot,
            N_Vector xdot_old,
            N_Vector * sx,
            TempData * tdata ) [virtual]
```

Sensitivity update functions for events, total derivative

Definition at line 113 of file amici_model.h.

Here is the caller graph for this function:



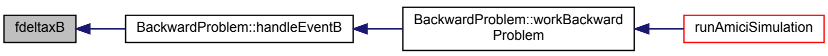
9.10.2.28 fdeltaxB()

```
virtual int fdeltaxB (
            realtype t,
            int ie,
            N_Vector x,
            N_Vector xB,
            N_Vector xdot,
            N_Vector xdot_old,
            TempData * tdata ) [virtual]
```

Adjoint state update functions for events

Definition at line 116 of file amici_model.h.

Here is the caller graph for this function:



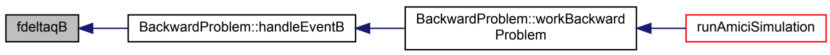
9.10.2.29 fdeltaqB()

```
virtual int fdeltaqB (
            realtype t,
            int ie,
            N_Vector x,
            N_Vector xB,
            N_Vector qBdot,
            N_Vector xdot,
            N_Vector xdot_old,
            TempData * tdata ) [virtual]
```

Quadrature state update functions for events

Definition at line 119 of file amici_model.h.

Here is the caller graph for this function:



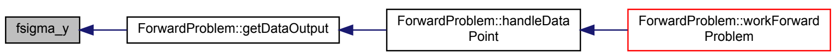
9.10.2.30 fsigma_y()

```
virtual int fsigma_y (
            realtype t,
            TempData * tdata ) [virtual]
```

Standard deviation of measurements

Definition at line 122 of file amici_model.h.

Here is the caller graph for this function:



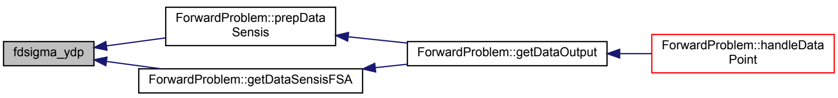
9.10.2.31 fdsigma_ydp()

```
virtual int fdsigma_ydp (
            realtype t,
            TempData * tdata )  [virtual]
```

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

Definition at line 125 of file amici_model.h.

Here is the caller graph for this function:



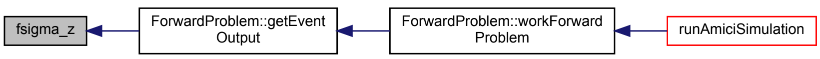
9.10.2.32 fsigma_z()

```
virtual int fsigma_z (
            realtype t,
            int ie,
            TempData * tdata )  [virtual]
```

Standard deviation of events

Definition at line 128 of file amici_model.h.

Here is the caller graph for this function:



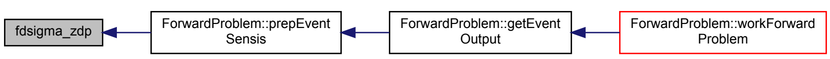
9.10.2.33 fdsigma_zdp()

```
virtual int fdsigma_zdp (
            realtype t,
            int ie,
            TempData * tdata )  [virtual]
```

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

Definition at line 131 of file amici_model.h.

Here is the caller graph for this function:



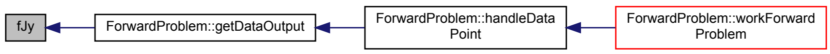
9.10.2.34 fJy()

```
virtual int fJy (
            realtype t,
            int it,
            N_Vector x,
            TempData * tdata,
            const ExpData * edata,
            ReturnData * rdata ) [virtual]
```

negative log-likelihood of time-resolved measurements y

Definition at line 134 of file amici_model.h.

Here is the caller graph for this function:



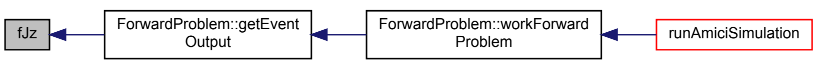
9.10.2.35 fJz()

```
virtual int fJz (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata,
            const ExpData * edata,
            ReturnData * rdata ) [virtual]
```

negative log-likelihood of event-resolved measurements z

Definition at line 137 of file amici_model.h.

Here is the caller graph for this function:



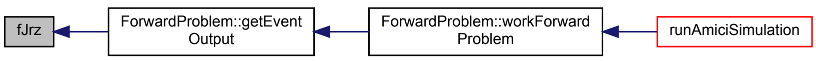
9.10.2.36 fJrz()

```
virtual int fJrz (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata,
            const ExpData * edata,
            ReturnData * rdata ) [virtual]
```

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

Definition at line 140 of file amici_model.h.

Here is the caller graph for this function:



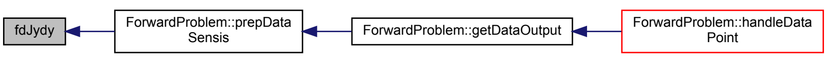
9.10.2.37 fdJydy()

```
virtual int fdJydy (
            realtype t,
            int it,
            N_Vector x,
            TempData * tdata,
            const ExpData * edata,
            ReturnData * rdata ) [virtual]
```

Sensitivity of time-resolved measurement negative log-likelihood Jy w.r.t. observables y

Definition at line 143 of file amici_model.h.

Here is the caller graph for this function:



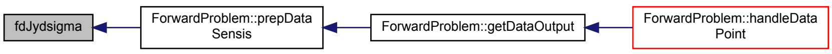
9.10.2.38 fdJydsigma()

```
virtual int fdJydsigma (
            realtype t,
            int it,
            N_Vector x,
            TempData * tdata,
            const ExpData * edata,
            ReturnData * rdata )  [virtual]
```

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

Definition at line 146 of file amici_model.h.

Here is the caller graph for this function:



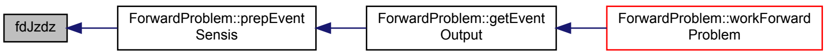
9.10.2.39 fdJzdz()

```
virtual int fdJzdz (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata,
            const ExpData * edata,
            ReturnData * rdata )  [virtual]
```

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

Definition at line 149 of file amici_model.h.

Here is the caller graph for this function:



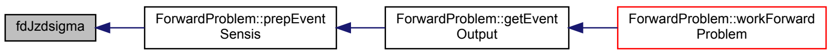
9.10.2.40 fdJzdsigma()

```
virtual int fdJzdsigma (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata,
            const ExpData * edata,
            ReturnData * rdata ) [virtual]
```

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

Definition at line 152 of file amici_model.h.

Here is the caller graph for this function:



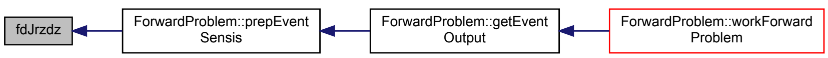
9.10.2.41 fdJrzdz()

```
virtual int fdJrzdz (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata,
            const ExpData * edata,
            ReturnData * rdata ) [virtual]
```

Sensitivity of event-resolved measurement negative log-likelihood regularization Jrz w.r.t. event observables z

Definition at line 155 of file amici_model.h.

Here is the caller graph for this function:



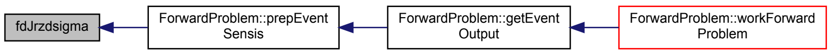
9.10.2.42 fdJrzdsigma()

```
virtual int fdJrzdsigma (
            realtype t,
            int ie,
            N_Vector x,
            TempData * tdata,
            const ExpData * edata,
            ReturnData * rdata ) [virtual]
```

Sensitivity of event-resolved measurement negative log-likelihood regularization Jrz w.r.t. standard deviation sigma

Definition at line 158 of file amici_model.h.

Here is the caller graph for this function:



9.10.2.43 fsxdot()

```
virtual int fsxdot (
            int Ns,
            realtype t,
            N_Vector x,
            N_Vector xdot,
            int ip,
            N_Vector sx,
            N_Vector sxdot,
            void * user_data,
            N_Vector tmp1,
            N_Vector tmp2 ) [virtual]
```

Right hand side of differential equation for state sensitivities sx

Definition at line 161 of file amici_model.h.

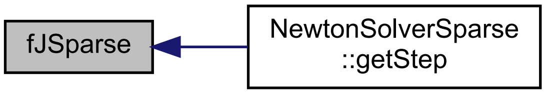
9.10.2.44 fJSparse()

```
virtual int fJSparse (
            realtype t,
            N_Vector x,
            N_Vector xdot,
            SlsMat J,
            void * user_data,
            N_Vector tmp1,
            N_Vector tmp2,
            N_Vector tmp3 ) [virtual]
```

J in sparse form (for sparse solvers from the SuiteSparse Package)

Definition at line 164 of file amici_model.h.

Here is the caller graph for this function:



9.10.2.45 fJBand()

```
virtual int fJBand (
            long int N,
            long int mupper,
            long int mlower,
            realtype t,
            N_Vector x,
            N_Vector xdot,
            DlsMat J,
            void * user_data,
            N_Vector tmp1,
            N_Vector tmp2,
            N_Vector tmp3 )  [virtual]
```

J in banded form (for banded solvers)

Definition at line 167 of file amici_model.h.

9.10.2.46 fJBandB()

```
virtual int fJBandB (
            long int NeqBdot,
            long int mupper,
            long int mlower,
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector xBdot,
            DlsMat JB,
            void * user_data,
            N_Vector tmp1B,
            N_Vector tmp2B,
            N_Vector tmp3B )  [virtual]
```

JB in banded form (for banded solvers)

Definition at line 170 of file amici_model.h.

9.10.2.47 fJvB()

```
virtual int fJvB (
            N_Vector vB,
            N_Vector JvB,
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector xBdot,
            void * user_data,
            N_Vector tmpB ) [virtual]
```

Matrix vector product of JB with a vector v (for iterative solvers)

Definition at line 173 of file amici_model.h.

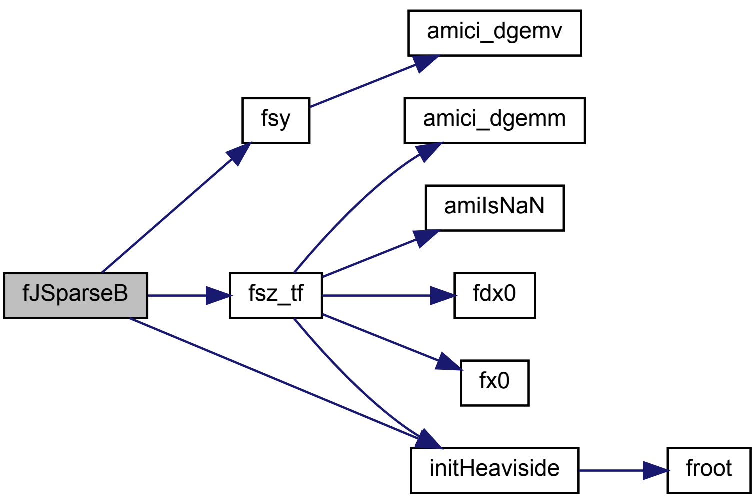
9.10.2.48 fJSparseB()

```
virtual int fJSparseB (
            realtype t,
            N_Vector x,
            N_Vector xB,
            N_Vector xBdot,
            SlsMat JB,
            void * user_data,
            N_Vector tmp1B,
            N_Vector tmp2B,
            N_Vector tmp3B ) [virtual]
```

JB in sparse form (for sparse solvers from the SuiteSparse Package)

Definition at line 176 of file amici_model.h.

Here is the call graph for this function:



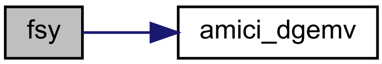
9.10.2.49 fsy()

```
int fsy (
            int it,
            TempData * tdata,
            ReturnData * rdata )
```

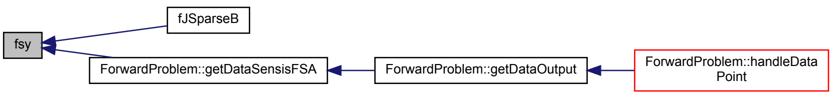
Sensitivity of measurements y, total derivative

Definition at line 24 of file amici_model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



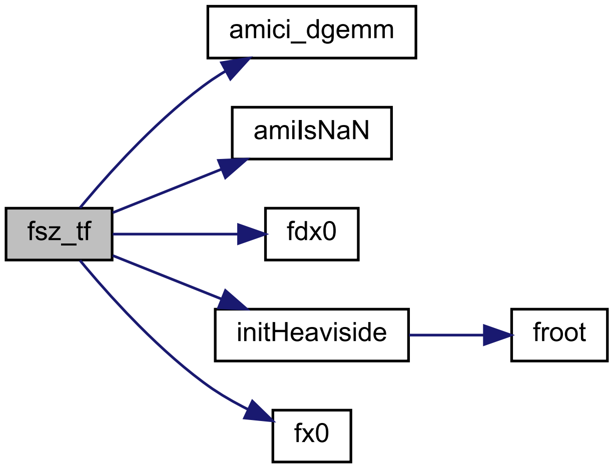
9.10.2.50 fsz_tf()

```
int fsz_tf (
            int ie,
            TempData * tdata,
            ReturnData * rdata )
```

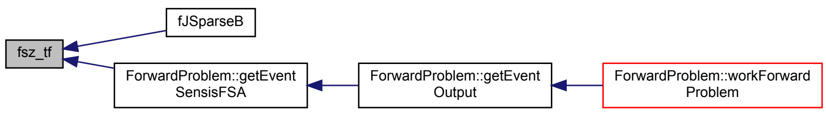
Sensitivity of z at final timepoint (ignores sensitivity of timepoint), total derivative

Definition at line 46 of file amici_model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.10.2.51 initHeaviside()

```
int initHeaviside (
            TempData * tdata )
```

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

Parameters

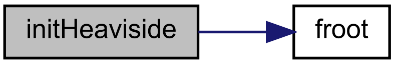
out	*tdata*	pointer to the temporary data struct **Type**: TempData

Returns

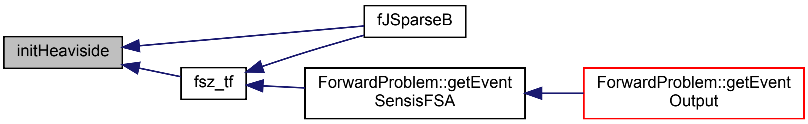
status flag indicating success of execution
Type: int

Definition at line 402 of file amici_model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.10.3 Member Data Documentation

9.10.3.1 np

```
const int np
```

total number of model parameters

Definition at line 217 of file amici_model.h.

9.10.3.2 nk

```
const int nk
```

number of fixed parameters

Definition at line 219 of file amici_model.h.

9.10.3.3 nx

```
const int nx
```

number of states

Definition at line 221 of file amici_model.h.

9.10.3.4 nxtrue

```
const int nxtrue
```

number of states in the unaugmented system

Definition at line 223 of file amici_model.h.

9.10.3.5 ny

```
const int ny
```

number of observables

Definition at line 225 of file amici_model.h.

9.10.3.6 nytrue

```
const int nytrue
```

number of observables in the unaugmented system

Definition at line 227 of file amici_model.h.

9.10.3.7 nz

```
const int nz
```

number of event outputs

Definition at line 229 of file amici_model.h.

9.10.3.8 nztrue

```
const int nztrue
```

number of event outputs in the unaugmented system

Definition at line 231 of file amici_model.h.

9.10.3.9 ne

```
const int ne
```

number of events

Definition at line 233 of file amici_model.h.

9.10.3.10 nw

```
const int nw
```

number of common expressions

Definition at line 235 of file amici_model.h.

9.10.3.11 ndwdx

```
const int ndwdx
```

number of derivatives of common expressions wrt x

Definition at line 237 of file amici_model.h.

9.10.3.12 ndwdp

```
const int ndwdp
```

number of derivatives of common expressions wrt p

Definition at line 239 of file amici_model.h.

9.10.3.13 nnz

```
const int nnz
```

number of nonzero entries in jacobian

Definition at line 241 of file amici_model.h.

9.10.3.14 nJ

```
const int nJ
```

dimension of the augmented objective function for 2nd order ASA

Definition at line 243 of file amici_model.h.

9.10.3.15 ubw

```
const int ubw
```

upper bandwith of the jacobian

Definition at line 245 of file amici_model.h.

9.10.3.16 lbw

```
const int lbw
```

lower bandwith of the jacobian

Definition at line 247 of file amici_model.h.

9.10.3.17 o2mode

```
const AMICI_o2mode o2mode
```

flag indicating whether for sensi == AMICI_SENSI_ORDER_SECOND directional or full second order derivative will be computed

Definition at line 250 of file amici_model.h.

9.10.3.18 z2event

```
int* z2event = nullptr
```

index indicating to which event an event output belongs

Definition at line 252 of file amici_model.h.

9.10.3.19 idlist

```
realtype* idlist = nullptr
```

flag array for DAE equations

Definition at line 254 of file amici_model.h.

9.11 modelTest Class Reference

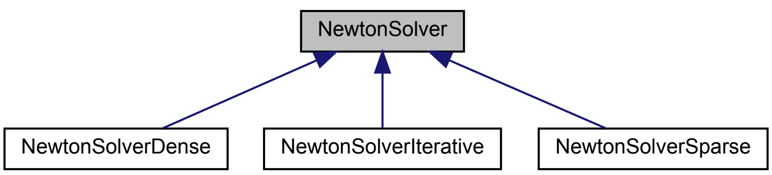
MODELTEST Summary of this class goes here Detailed explanation goes here.

9.11.1 Detailed Description

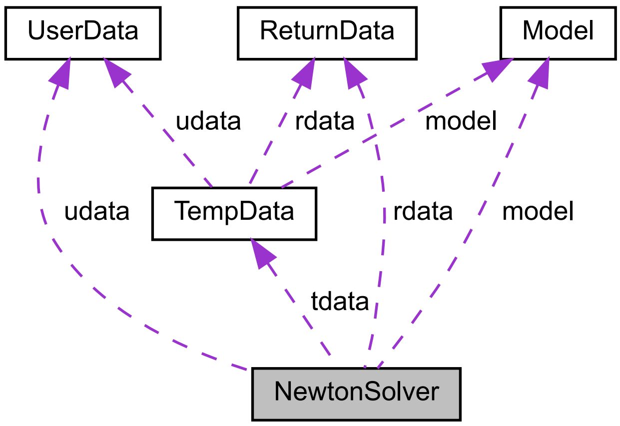
Definition at line 17 of file modelTest.m.

9.12 NewtonSolver Class Reference

Inheritance diagram for NewtonSolver:



Collaboration diagram for NewtonSolver:



Public Member Functions

- **NewtonSolver** (Model *model, ReturnData *rdata, UserData *udata, TempData *tdata)
- virtual int getStep (int ntry, int nnewt, N_Vector delta)=0

Static Public Member Functions

- static NewtonSolver * getSolver (int linsolType, Model *model, ReturnData *rdata, UserData *udata, TempData *tdata, int *status)

Protected Attributes

- Model * **model**
- ReturnData * **rdata**
- UserData * **udata**
- TempData * **tdata**

9.12.1 Detailed Description

Definition at line 17 of file newton_solver.h.

9.12.2 Member Function Documentation

9.12.2.1 getSolver()

```
NewtonSolver * getSolver (
              int linsolType,
              Model * model,
              ReturnData * rdata,
              UserData * udata,
              TempData * tdata,
              int * status ) [static]
```

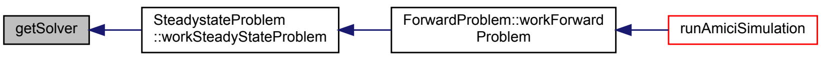
getNewtonStep computes the Newton Step by solving the linear system

Parameters

in	*udata*	pointer to the user data struct **Type**: UserData
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*tdata*	pointer to the temporary data struct **Type**: TempData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
out	*status*	flag indicating success of execution **Type**: int

Definition at line 18 of file newton_solver.cpp.

Here is the caller graph for this function:



9.12.2.2 getStep()

```
virtual int getStep (
              int ntry,
              int nnewt,
              N_Vector delta ) [pure virtual]
```

Parameters

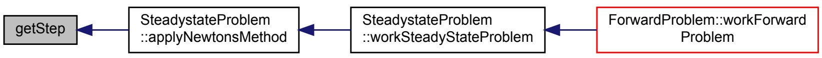
in	*ntry*	integer number of Newton solver try
in	*nnewt*	integer number of Newton steps in the current Newton solver try
out	*delta*	N_Vector solution of the linear system

Returns

int status flag indicating success of execution
Type: int

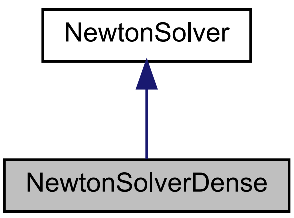
Implemented in NewtonSolverIterative, NewtonSolverSparse, and NewtonSolverDense.

Here is the caller graph for this function:

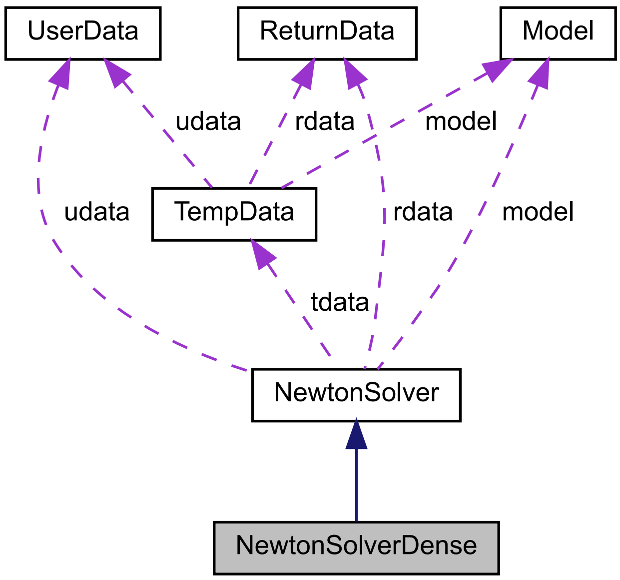


9.13 NewtonSolverDense Class Reference

Inheritance diagram for NewtonSolverDense:



Collaboration diagram for NewtonSolverDense:



Public Member Functions

- **NewtonSolverDense** (Model ∗model, ReturnData ∗rdata, UserData ∗udata, TempData ∗tdata)
- int getStep (int ntry, int nnewt, N_Vector delta)

Additional Inherited Members

9.13.1 Detailed Description

Definition at line 42 of file newton_solver.h.

9.13.2 Member Function Documentation

9.13.2.1 getStep()

```
int getStep (
            int ntry,
            int nnewt,
            N_Vector delta )  [virtual]
```

Parameters

in	*ntry*	integer number of Newton solver try
in	*nnewt*	integer number of Newton steps in the current Newton solver try
out	*delta*	N_Vector solution of the linear system

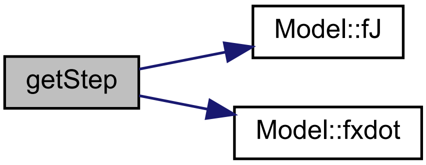
Returns

int status flag indicating success of execution
Type: int

Implements NewtonSolver.

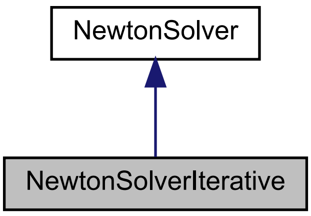
Definition at line 95 of file newton_solver.cpp.

Here is the call graph for this function:

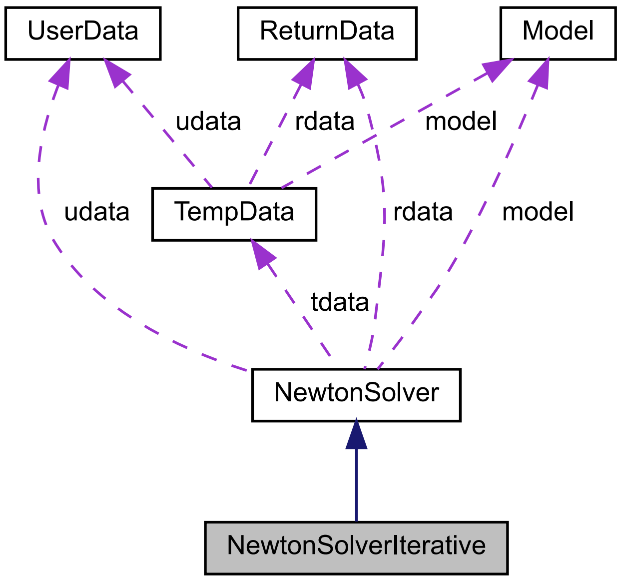


9.14 NewtonSolverIterative Class Reference

Inheritance diagram for NewtonSolverIterative:



Collaboration diagram for NewtonSolverIterative:



Public Member Functions

- **NewtonSolverIterative** (Model ∗model, ReturnData ∗rdata, UserData ∗udata, TempData ∗tdata)
- int getStep (int ntry, int nnewt, N_Vector delta)

Additional Inherited Members

9.14.1 Detailed Description

Definition at line 77 of file newton_solver.h.

9.14.2 Member Function Documentation

9.14.2.1 getStep()

```
int getStep (
            int ntry,
            int nnewt,
            N_Vector delta )  [virtual]
```

Parameters

`in`	*ntry*	integer number of Newton solver try
`in`	*nnewt*	integer number of Newton steps in the current Newton solver try
`out`	*delta*	N_Vector solution of the linear system

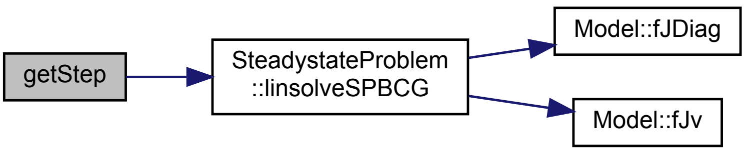
Returns

int status flag indicating success of execution
Type: int

Implements NewtonSolver.

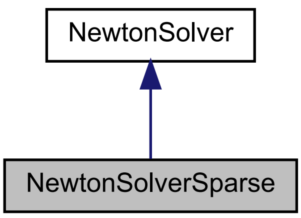
Definition at line 189 of file newton_solver.cpp.

Here is the call graph for this function:

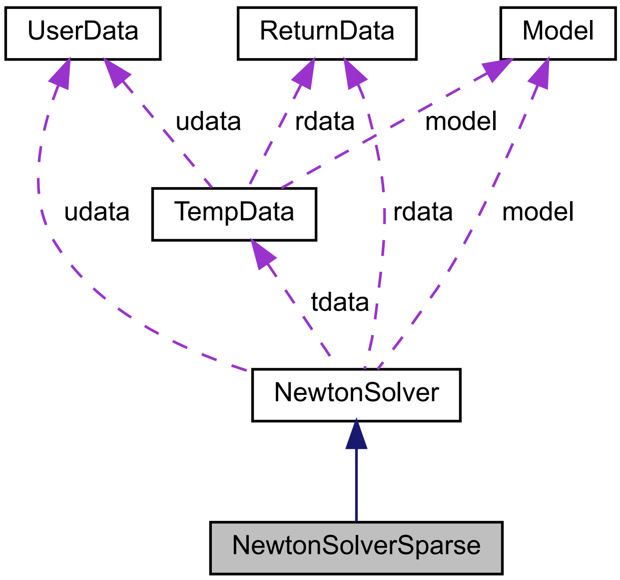


9.15 NewtonSolverSparse Class Reference

Inheritance diagram for NewtonSolverSparse:



Collaboration diagram for NewtonSolverSparse:



Public Member Functions

- **NewtonSolverSparse** (Model *model, ReturnData *rdata, UserData *udata, TempData *tdata)
- int getStep (int ntry, int nnewt, N_Vector delta)

Additional Inherited Members

9.15.1 Detailed Description

Definition at line 58 of file newton_solver.h.

9.15.2 Member Function Documentation

9.15.2.1 getStep()

```
int getStep (
            int ntry,
            int nnewt,
            N_Vector delta )  [virtual]
```

Parameters

in	*ntry*	integer number of Newton solver try
in	*nnewt*	integer number of Newton steps in the current Newton solver try
out	*delta*	N_Vector solution of the linear system

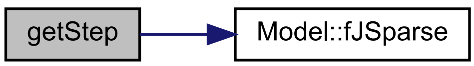
Returns

int status flag indicating success of execution
Type: int

Implements NewtonSolver.

Definition at line 142 of file newton_solver.cpp.

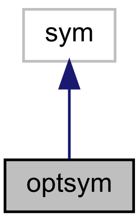
Here is the call graph for this function:



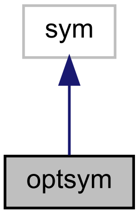
9.16 optsym Class Reference

OPTSYM is an auxiliary class to gain access to the private symbolic property `s` which is necessary to be able to call symobj::optimize on it.

Inheritance diagram for optsym:



Collaboration diagram for optsym:



Public Member Functions

- optsym (::sym symbol)

  optsym converts the symbolic object into a optsym object
- mlhsInnerSubst<::sym > getoptimized ()

  getoptimized calls symobj::optimize on the optsym object

9.16.1 Detailed Description

Definition at line 17 of file optsym.m.

9.16.2 Constructor & Destructor Documentation

9.16.2.1 optsym()

```
optsym (
            ::sym symbol )
```

Parameters

symbol	symbolic object

Definition at line 32 of file optsym.m.

9.16.3 Member Function Documentation

9.16.3.1 getoptimized()

```
mlhsInnerSubst<::sym > getoptimized ( )
```

Return values

out	optimized symbolic object

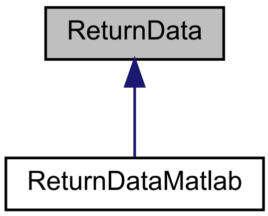
Definition at line 42 of file optsym.m.

9.17 ReturnData Class Reference

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

`#include <rdata.h>`

Inheritance diagram for ReturnData:



Public Member Functions

- ReturnData ()
  default constructor
- ReturnData (const UserData *udata, const Model *model)
- virtual void setDefaults ()
- void invalidate ()
- void setLikelihoodSensitivityFirstOrderNaN ()
- void setLikelihoodSensitivitySecondOrderNaN ()
- int applyChainRuleFactorToSimulationResults (const UserData *udata, const realtype *unscaledParameters)
- virtual ~ReturnData ()

Public Attributes

- double * ts
- double * xdot
- double * dxdotdp
- double * dydx
- double * dydp
- double * J
- double * z
- double * sigmaz

- double ∗ sz
- double ∗ ssigmaz
- double ∗ rz
- double ∗ srz
- double ∗ s2rz
- double ∗ x
- double ∗ sx
- double ∗ y
- double ∗ sigmay
- double ∗ sy
- double ∗ ssigmay
- double ∗ numsteps
- double ∗ numstepsB
- double ∗ numrhsevals
- double ∗ numrhsevalsB
- double ∗ numerrtestfails
- double ∗ numerrtestfailsB
- double ∗ numnonlinsolvconvfails
- double ∗ numnonlinsolvconvfailsB
- double ∗ order
- double ∗ newton_status
- double ∗ newton_time
- double ∗ newton_numsteps
- double ∗ newton_numlinsteps
- double ∗ xss
- double ∗ llh
- double ∗ chi2
- double ∗ sllh
- double ∗ s2llh
- double ∗ status
- const int np
- const int nk
- const int nx
- 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
- const AMICI_parameter_scaling pscale
- const AMICI_o2mode o2mode
- const AMICI_sensi_order sensi
- const AMICI_sensi_meth sensi_meth

Protected Member Functions

- virtual void copyFromUserData (const UserData ∗udata)
- virtual void initFields ()
- virtual void initField1 (double ∗∗fieldPointer, const char ∗fieldName, int dim)
- virtual void initField2 (double ∗∗fieldPointer, const char ∗fieldName, int dim1, int dim2)
- virtual void initField3 (double ∗∗fieldPointer, const char ∗fieldName, int dim1, int dim2, int dim3)
- virtual void initField4 (double ∗∗fieldPointer, const char ∗fieldName, int dim1, int dim2, int dim3, int dim4)

Protected Attributes

- bool freeFieldsOnDestruction

9.17.1 Detailed Description

NOTE: MATLAB stores multidimensional arrays in column-major order (FORTRAN-style)

Definition at line 13 of file rdata.h.

9.17.2 Constructor & Destructor Documentation

9.17.2.1 ReturnData()

```
ReturnData (
              const UserData * udata,
              const Model * model )
```

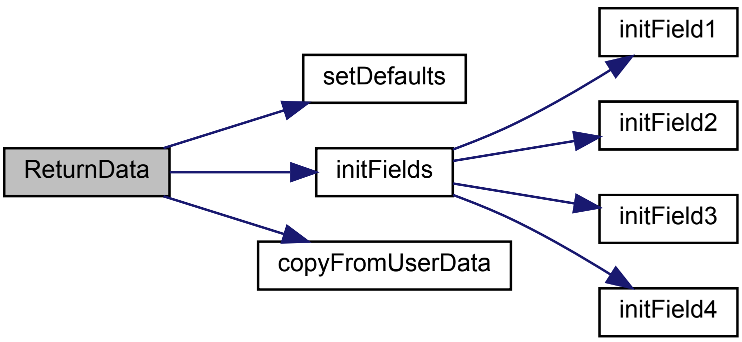
constructor that uses information from model and userdata to appropriately initialize fields

Parameters

in	*udata*	pointer to the user data struct **Type**: UserData
in	*model*	pointer to model specification object **Type**: Model

Definition at line 19 of file rdata.cpp.

Here is the call graph for this function:



9.17.2.2 ∼ReturnData()

```
~ReturnData ( ) [virtual]
```

default destructor

Definition at line 268 of file rdata.cpp.

9.17.3 Member Function Documentation

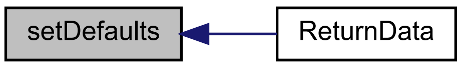
9.17.3.1 setDefaults()

```
void setDefaults ( ) [virtual]
```

initialize all member fields will nullpointers

Definition at line 40 of file rdata.cpp.

Here is the caller graph for this function:



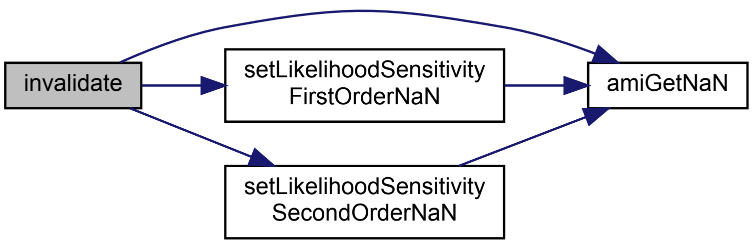
9.17.3.2 invalidate()

```
void invalidate ( )
```

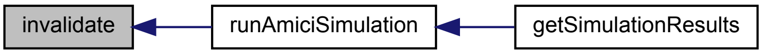
routine to set likelihood and respective sensitivities to NaN (typically after integration failure)

Definition at line 57 of file rdata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



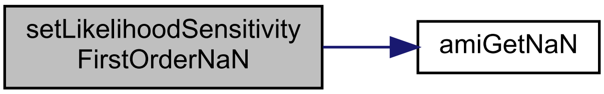
9.17.3.3 setLikelihoodSensitivityFirstOrderNaN()

```
void setLikelihoodSensitivityFirstOrderNaN ( )
```

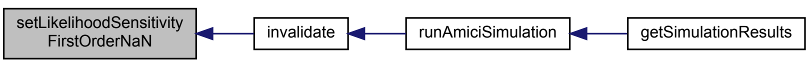
routine to set first order sensitivities to NaN (typically after integration failure)

Definition at line 71 of file rdata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



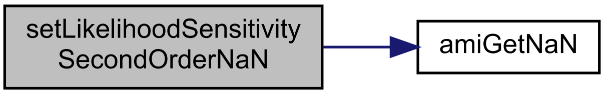
9.17.3.4 setLikelihoodSensitivitySecondOrderNaN()

```
void setLikelihoodSensitivitySecondOrderNaN ( )
```

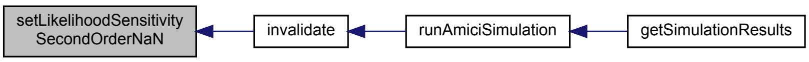
routine to set second order sensitivities to NaN (typically after integration failure)

Definition at line 78 of file rdata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.17.3.5 applyChainRuleFactorToSimulationResults()

```
int applyChainRuleFactorToSimulationResults (
            const UserData * udata,
            const realtype * unscaledParameters )
```

applies the chain rule to account for parameter transformation in the sensitivities of simulation results

Parameters

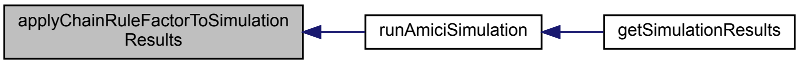
in	*udata*	pointer to the user data struct **Type**: UserData
in	*unscaledParameters*	pointer to the non-transformed parameters **Type**: realtype

Returns

status flag indicating success of execution
Type: int

Definition at line 85 of file rdata.cpp.

Here is the caller graph for this function:



9.17.3.6 copyFromUserData()

```
void copyFromUserData (
            const UserData * udata )  [protected], [virtual]
```

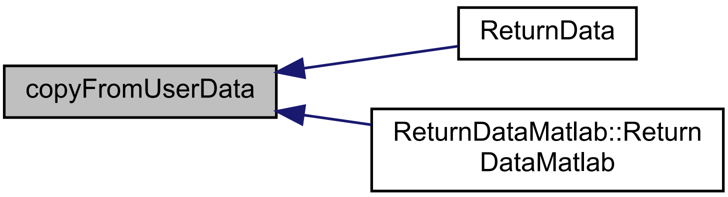
copies measurement timepoints from UserData object

Parameters

in	*udata*	pointer to the user data struct **Type**: UserData

Definition at line 353 of file rdata.cpp.

Here is the caller graph for this function:



9.17.3.7 initFields()

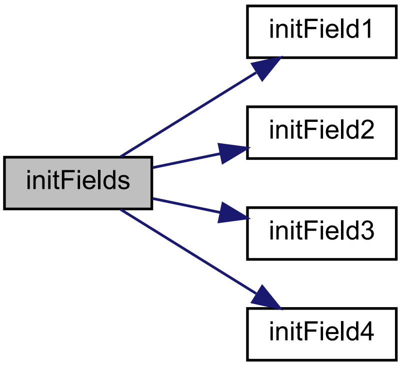
```
void initFields ( )  [protected], [virtual]
```

initialises sol object with the corresponding fields

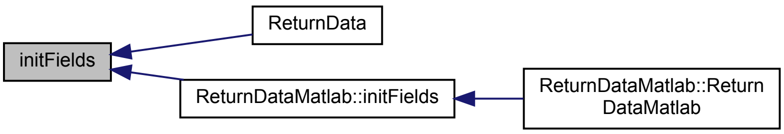
Reimplemented in ReturnDataMatlab.

Definition at line 361 of file rdata.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.17.3.8 initField1()

```
void initField1 (
            double ** fieldPointer,
            const char * fieldName,
            int dim )  [protected], [virtual]
```

initialise vector and attach to the field

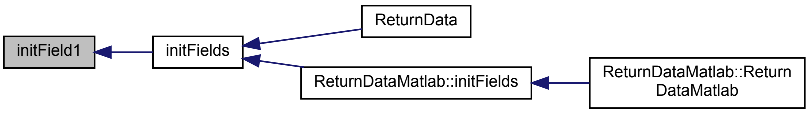
Parameters

fieldPointer	pointer of the field to which the vector will be attached
fieldName	Name of the field to which the vector will be attached
dim	number of elements in the vector

Reimplemented in ReturnDataMatlab.

Definition at line 441 of file rdata.cpp.

Here is the caller graph for this function:



9.17.3.9 initField2()

```
void initField2 (
            double ** fieldPointer,
            const char * fieldName,
            int dim1,
            int dim2 )  [protected], [virtual]
```

initialise matrix and attach to the field

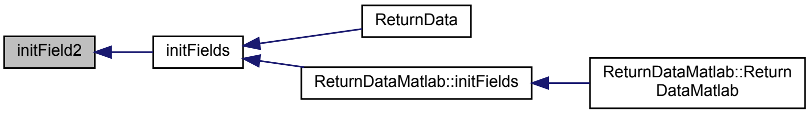
Parameters

fieldPointer	pointer of the field to which the matrix will be attached
fieldName	Name of the field to which the matrix will be attached
dim1	number of rows in the matrix
dim2	number of columns in the matrix

Reimplemented in ReturnDataMatlab.

Definition at line 452 of file rdata.cpp.

Here is the caller graph for this function:



9.17.3.10 initField3()

```
void initField3 (
            double ** fieldPointer,
            const char * fieldName,
            int dim1,
            int dim2,
            int dim3 )  [protected], [virtual]
```

initialise 3D tensor and attach to the field

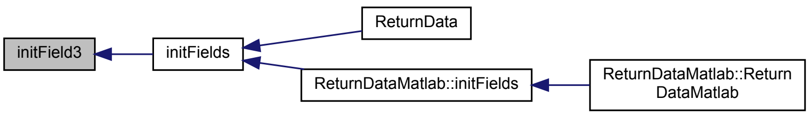
Parameters

fieldPointer	pointer of the field to which the tensor will be attached
fieldName	Name of the field to which the tensor will be attached
dim1	number of rows in the tensor
dim2	number of columns in the tensor
dim3	number of elements in the third dimension of the tensor

Reimplemented in ReturnDataMatlab.

Definition at line 464 of file rdata.cpp.

Here is the caller graph for this function:



9.17.3.11 initField4()

```
void initField4 (
            double ** fieldPointer,
            const char * fieldName,
            int dim1,
            int dim2,
            int dim3,
            int dim4 )  [protected], [virtual]
```

initialise 4D tensor and attach to the field

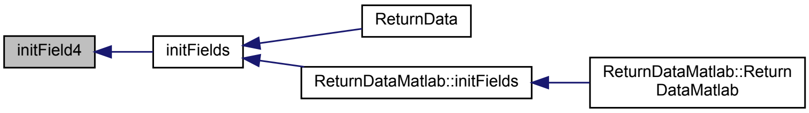
Parameters

fieldPointer	pointer of the field to which the tensor will be attached
fieldName	Name of the field to which the tensor will be attached
dim1	number of rows in the tensor
dim2	number of columns in the tensor
dim3	number of elements in the third dimension of the tensor
dim4	number of elements in the fourth dimension of the tensor

Reimplemented in ReturnDataMatlab.

Definition at line 478 of file rdata.cpp.

Here is the caller graph for this function:



9.17.4 Member Data Documentation

9.17.4.1 ts

```
double* ts
```

timepoints (dimension: nt)

Definition at line 33 of file rdata.h.

9.17.4.2 xdot

```
double* xdot
```

time derivative (dimension: nx)

Definition at line 36 of file rdata.h.

9.17.4.3 dxdotdp

```
double* dxdotdp
```

parameter derivative of time derivative (dimension: nx x nplist, column-major)

Definition at line 40 of file rdata.h.

9.17.4.4 dydx

```
double* dydx
```

state derivative of observables (dimension: ny x nx, column-major)

Definition at line 43 of file rdata.h.

9.17.4.5 dydp

```
double* dydp
```

parameter derivative of observables (dimension: ny x nplist, column-major)

Definition at line 47 of file rdata.h.

9.17.4.6 J

```
double* J
```

Jacobian of differential equation right hand side (dimension: nx x nx, column-major)

Definition at line 51 of file rdata.h.

9.17.4.7 z

```
double* z
```

event output (dimension: nmaxevent x nz, column-major)

Definition at line 54 of file rdata.h.

9.17.4.8 sigmaz

```
double* sigmaz
```

event output sigma standard deviation (dimension: nmaxevent x nz, column-major)

Definition at line 58 of file rdata.h.

9.17.4.9 sz

```
double* sz
```

parameter derivative of event output (dimension: nmaxevent x nz, column-major)

Definition at line 62 of file rdata.h.

9.17.4.10 ssigmaz

```
double* ssigmaz
```

parameter derivative of event output standard deviation (dimension: nmaxevent x nz, column-major)

Definition at line 66 of file rdata.h.

9.17.4.11 rz

```
double* rz
```

event trigger output (dimension: nmaxevent x nz, column-major)

Definition at line 69 of file rdata.h.

9.17.4.12 srz

```
double* srz
```

parameter derivative of event trigger output (dimension: nmaxevent x nz x nplist, column-major)

Definition at line 73 of file rdata.h.

9.17.4.13 s2rz

```
double* s2rz
```

second order parameter derivative of event trigger output (dimension: nmaxevent x nztrue x nplist x nplist, column-major)

Definition at line 77 of file rdata.h.

9.17.4.14 x

```
double* x
```

state (dimension: nt x nx, column-major)

Definition at line 80 of file rdata.h.

9.17.4.15 sx

```
double* sx
```

parameter derivative of state (dimension: nt x nx x nplist, column-major)

Definition at line 84 of file rdata.h.

9.17.4.16 y

```
double* y
```

observable (dimension: nt x ny, column-major)

Definition at line 87 of file rdata.h.

9.17.4.17 sigmay

```
double* sigmay
```

observable standard deviation (dimension: nt x ny, column-major)

Definition at line 90 of file rdata.h.

9.17.4.18 sy

```
double* sy
```

parameter derivative of observable (dimension: nt x ny x nplist, column-major)

Definition at line 94 of file rdata.h.

9.17.4.19 ssigmay

```
double* ssigmay
```

parameter derivative of observable standard deviation (dimension: nt x ny x nplist, column-major)

Definition at line 98 of file rdata.h.

9.17.4.20 numsteps

```
double* numsteps
```

number of integration steps forward problem (dimension: nt)

Definition at line 101 of file rdata.h.

9.17.4.21 numstepsB

```
double* numstepsB
```

number of integration steps backward problem (dimension: nt)

Definition at line 104 of file rdata.h.

9.17.4.22 numrhsevals

```
double* numrhsevals
```

number of right hand side evaluations forward problem (dimension: nt)

Definition at line 107 of file rdata.h.

9.17.4.23 numrhsevalsB

```
double* numrhsevalsB
```

number of right hand side evaluations backwad problem (dimension: nt)

Definition at line 110 of file rdata.h.

9.17.4.24 numerrtestfails

`double* numerrtestfails`

number of error test failures forward problem (dimension: nt)

Definition at line 113 of file rdata.h.

9.17.4.25 numerrtestfailsB

`double* numerrtestfailsB`

number of error test failures backwad problem (dimension: nt)

Definition at line 116 of file rdata.h.

9.17.4.26 numnonlinsolvconvfails

`double* numnonlinsolvconvfails`

number of linear solver convergence failures forward problem (dimension: nt)

Definition at line 120 of file rdata.h.

9.17.4.27 numnonlinsolvconvfailsB

`double* numnonlinsolvconvfailsB`

number of linear solver convergence failures backwad problem (dimension: nt)

Definition at line 124 of file rdata.h.

9.17.4.28 order

`double* order`

employed order forward problem (dimension: nt)

Definition at line 127 of file rdata.h.

9.17.4.29 newton_status

```
double* newton_status
```

flag indicating success of Newton solver

Definition at line 130 of file rdata.h.

9.17.4.30 newton_time

```
double* newton_time
```

computation time of the Newton solver [s]

Definition at line 133 of file rdata.h.

9.17.4.31 newton_numsteps

```
double* newton_numsteps
```

number of Newton steps for steady state problem

Definition at line 136 of file rdata.h.

9.17.4.32 newton_numlinsteps

```
double* newton_numlinsteps
```

number of linear steps by Newton step for steady state problem

Definition at line 139 of file rdata.h.

9.17.4.33 xss

```
double* xss
```

steady state found be Newton solver

Definition at line 142 of file rdata.h.

9.17.4.34 llh

```
double* llh
```

likelihood value (double[1])

Definition at line 145 of file rdata.h.

9.17.4.35 chi2

```
double* chi2
```

chi2 value (double[1])

Definition at line 148 of file rdata.h.

9.17.4.36 sllh

```
double* sllh
```

parameter derivative of likelihood (dimension: nplist)

Definition at line 151 of file rdata.h.

9.17.4.37 s2llh

```
double* s2llh
```

second order parameter derivative of likelihood (dimension: (nJ-1) x nplist, column-major)

Definition at line 155 of file rdata.h.

9.17.4.38 status

```
double* status
```

status code (double[1])

Definition at line 158 of file rdata.h.

9.17.4.39 freeFieldsOnDestruction

```
bool freeFieldsOnDestruction [protected]
```

flag indicating whether memory for fields needs to be freed on destruction

Definition at line 178 of file rdata.h.

9.17.4.40 np

```
const int np
```

total number of model parameters

Definition at line 182 of file rdata.h.

9.17.4.41 nk

```
const int nk
```

number of fixed parameters

Definition at line 184 of file rdata.h.

9.17.4.42 nx

```
const int nx
```

number of states

Definition at line 186 of file rdata.h.

9.17.4.43 nxtrue

```
const int nxtrue
```

number of states in the unaugmented system

Definition at line 188 of file rdata.h.

9.17.4.44 ny

```
const int ny
```

number of observables

Definition at line 190 of file rdata.h.

9.17.4.45 nytrue

```
const int nytrue
```

number of observables in the unaugmented system

Definition at line 192 of file rdata.h.

9.17.4.46 nz

```
const int nz
```

number of event outputs

Definition at line 194 of file rdata.h.

9.17.4.47 nztrue

```
const int nztrue
```

number of event outputs in the unaugmented system

Definition at line 196 of file rdata.h.

9.17.4.48 ne

```
const int ne
```

number of events

Definition at line 198 of file rdata.h.

9.17.4.49 nJ

```
const int nJ
```

dimension of the augmented objective function for 2nd order ASA

Definition at line 200 of file rdata.h.

9.17.4.50 nplist

```
const int nplist
```

number of parameter for which sensitivities were requested

Definition at line 203 of file rdata.h.

9.17.4.51 nmaxevent

```
const int nmaxevent
```

maximal number of occuring events (for every event type)

Definition at line 205 of file rdata.h.

9.17.4.52 nt

```
const int nt
```

number of considered timepoints

Definition at line 207 of file rdata.h.

9.17.4.53 newton_maxsteps

```
const int newton_maxsteps
```

maximal number of newton iterations for steady state calculation

Definition at line 209 of file rdata.h.

9.17.4.54 pscale

```
const AMICI_parameter_scaling pscale
```

scaling of parameterization (lin,log,log10)

Definition at line 211 of file rdata.h.

9.17.4.55 o2mode

```
const AMICI_o2mode o2mode
```

flag indicating whether second order sensitivities were requested

Definition at line 213 of file rdata.h.

9.17.4.56 sensi

```
const AMICI_sensi_order sensi
```

sensitivity order

Definition at line 215 of file rdata.h.

9.17.4.57 sensi_meth

```
const AMICI_sensi_meth sensi_meth
```

sensitivity method

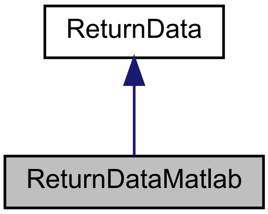
Definition at line 217 of file rdata.h.

9.18 ReturnDataMatlab Class Reference

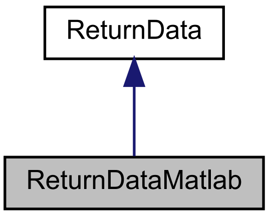
The ReturnDataMatlab class sets up ReturnData to be returned by the MATLAB mex functions. Memory is allocated using matlab functions.

`#include <returndata_matlab.h>`

Inheritance diagram for ReturnDataMatlab:



Collaboration diagram for ReturnDataMatlab:



Public Member Functions

- ReturnDataMatlab (const UserData *udata, const Model *model)

Public Attributes

- mxArray * **mxsol**

Protected Member Functions

- void initFields ()
- virtual void initField1 (double **fieldPointer, const char *fieldName, int dim)
- virtual void initField2 (double **fieldPointer, const char *fieldName, int dim1, int dim2)
- virtual void initField3 (double **fieldPointer, const char *fieldName, int dim1, int dim2, int dim3)
- virtual void initField4 (double **fieldPointer, const char *fieldName, int dim1, int dim2, int dim3, int dim4)

Additional Inherited Members

9.18.1 Detailed Description

Definition at line 15 of file returndata_matlab.h.

9.18.2 Constructor & Destructor Documentation

9.18.2.1 ReturnDataMatlab()

```
ReturnDataMatlab (
            const UserData * udata,
            const Model * model )
```

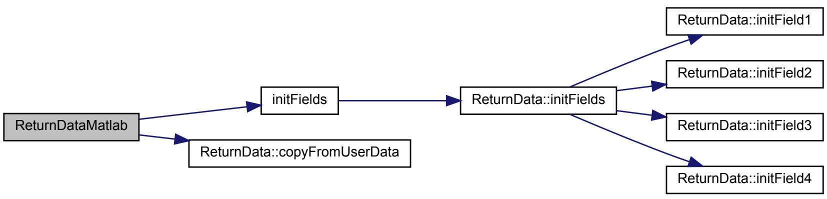
initialises the returnData struct, initialises the fields and copies model dimensions from the udata struct

Parameters

in	*udata*	pointer to the user data struct **Type**: UserData
in	*model*	pointer to model specification object **Type**: Model

Definition at line 3 of file returndata_matlab.cpp.

Here is the call graph for this function:



9.18.3 Member Function Documentation

9.18.3.1 initFields()

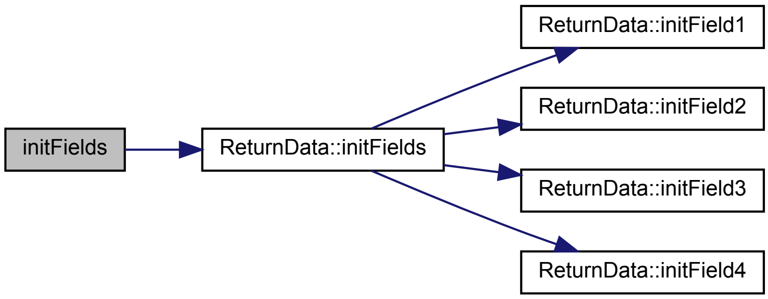
```
void initFields ( )  [protected], [virtual]
```

initialises sol object with the corresponding fields

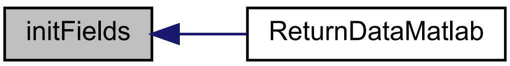
Reimplemented from ReturnData.

Definition at line 17 of file returndata_matlab.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.18.3.2 initField1()

```
void initField1 (
            double ** fieldPointer,
            const char * fieldName,
            int dim )  [protected], [virtual]
```

@ brief initialise vector and attach to the field @ param fieldPointer pointer of the field to which the vector will be attached @ param fieldName Name of the field to which the vector will be attached @ param dim number of elements in the vector initialise vector and attach to the field

Parameters

fieldPointer	pointer of the field to which the vector will be attached
fieldName	Name of the field to which the vector will be attached
dim	number of elements in the vector

Reimplemented from ReturnData.

Definition at line 66 of file returndata_matlab.cpp.

9.18.3.3 initField2()

```
void initField2 (
            double ** fieldPointer,
            const char * fieldName,
            int dim1,
            int dim2 ) [protected], [virtual]
```

@ brief initialise matrix and attach to the field @ param fieldPointer pointer of the field to which the matrix will be attached @ param fieldName Name of the field to which the matrix will be attached @ param dim1 number of rows in the matrix @ param dim2 number of columns in the matrix initialise matrix and attach to the field

Parameters

fieldPointer	pointer of the field to which the matrix will be attached
fieldName	Name of the field to which the matrix will be attached
dim1	number of rows in the matrix
dim2	number of columns in the matrix

Reimplemented from ReturnData.

Definition at line 83 of file returndata_matlab.cpp.

9.18.3.4 initField3()

```
void initField3 (
            double ** fieldPointer,
            const char * fieldName,
            int dim1,
            int dim2,
            int dim3 ) [protected], [virtual]
```

@ brief initialise 3D tensor and attach to the field @ param fieldPointer pointer of the field to which the tensor will be attached @ param fieldName Name of the field to which the tensor will be attached @ param dim1 number of rows in the tensor @ param dim2 number of columns in the tensor @ param dim3 number of elements in the third dimension of the tensor initialise 3D tensor and attach to the field

Parameters

fieldPointer	pointer of the field to which the tensor will be attached
fieldName	Name of the field to which the tensor will be attached
dim1	number of rows in the tensor
dim2	number of columns in the tensor
dim3	number of elements in the third dimension of the tensor

Reimplemented from ReturnData.

Definition at line 101 of file returndata_matlab.cpp.

9.18.3.5 initField4()

```
void initField4 (
            double ** fieldPointer,
            const char * fieldName,
            int dim1,
            int dim2,
            int dim3,
            int dim4 )  [protected], [virtual]
```

@ brief initialise 4D tensor and attach to the field @ param fieldPointer pointer of the field to which the tensor will be attached @ param fieldName Name of the field to which the tensor will be attached @ param dim1 number of rows in the tensor @ param dim2 number of columns in the tensor @ param dim3 number of elements in the third dimension of the tensor @ param dim4 number of elements in the fourth dimension of the tensor initialise 4D tensor and attach to the field

Parameters

fieldPointer	pointer of the field to which the tensor will be attached
fieldName	Name of the field to which the tensor will be attached
dim1	number of rows in the tensor
dim2	number of columns in the tensor
dim3	number of elements in the third dimension of the tensor
dim4	number of elements in the fourth dimension of the tensor

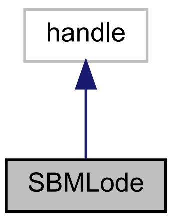
Reimplemented from ReturnData.

Definition at line 121 of file returndata_matlab.cpp.

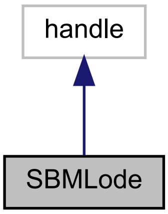
9.19 SBMLode Class Reference

SBMLMODEL provides an intermediate container between the SBML definition and an amimodel object.

Inheritance diagram for SBMLode:



Collaboration diagram for SBMLode:



Public Member Functions

- SBMLode (matlabtypesubstitute filename)

  SBMLode extracts information from an SBML definition and stores it in a symbolic format.
- noret::substitute checkODE (matlabtypesubstitute filename, matlabtypesubstitute this)

  checkODE checks whether the length of various variable names exceeds namelengthmax (would cause troube with symbolic processing later on).
- noret::substitute writeAMICI (matlabtypesubstitute modelname)

  writeAMICI writes the symbolic information from an SBMLode object into an AMICI model definition file

Public Attributes

- matlabtypesubstitute state = sym.empty("")

  states
- matlabtypesubstitute observable = sym.empty("")

  observables
- matlabtypesubstitute observable_name = sym.empty("")

  names of observables
- matlabtypesubstitute param = sym.empty("")

  parameter names
- matlabtypesubstitute parameter = sym.empty("")

  parameter expressions
- matlabtypesubstitute constant = sym.empty("")

  constants
- matlabtypesubstitute reaction = sym.empty("")

  reactions
- matlabtypesubstitute compartment = sym.empty("")

  compartments
- matlabtypesubstitute volume = sym.empty("")

  compartment volumes
- matlabtypesubstitute kvolume = sym.empty("")

  condition volumes
- matlabtypesubstitute initState = sym.empty("")

  initial condition of states
- matlabtypesubstitute condition = sym.empty("")

  condition
- matlabtypesubstitute flux = sym.empty("")

  reaction fluxes
- matlabtypesubstitute stochiometry = sym.empty("")

  reaction stochiometry
- matlabtypesubstitute xdot = sym.empty("")

  right hand side of reconstructed differential equation
- matlabtypesubstitute trigger = sym.empty("")

  event triggers
- matlabtypesubstitute bolus = sym.empty("")

  event boli
- matlabtypesubstitute funmath = cell.empty("")

  mathematical experessions for function
- matlabtypesubstitute **funarg** = cell.empty("")
- matlabtypesubstitute time_symbol = char.empty("")

  symbol of time
- matlabtypesubstitute pnom = double.empty("")

  nominal parameters
- matlabtypesubstitute knom = double.empty("")

  nominal conditions

9.19.1 Detailed Description

Definition at line 17 of file SBMLode.m.

9.19.2 Constructor & Destructor Documentation

9.19.2.1 SBMLode()

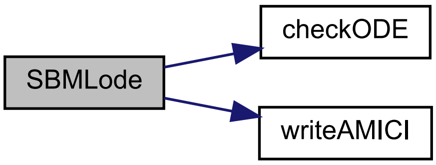
```
SBMLode (
        matlabtypesubstitute filename )
```

Parameters

filename	target name of the model (excluding the suffix .xml/.sbml)

Definition at line 201 of file SBMLode.m.

Here is the call graph for this function:



9.19.3 Member Function Documentation

9.19.3.1 writeAMICI()

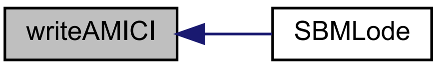
```
noret::substitute writeAMICI (
            matlabtypesubstitute modelname )
```

Parameters

modelname	target name of the model (_syms.m will be appended to the name)

Definition at line 18 of file writeAMICI.m.

Here is the caller graph for this function:



9.19.4 Member Data Documentation

9.19.4.1 state

```
state = sym.empty("")
```

Default: sym.empty("")

Definition at line 28 of file SBMLode.m.

9.19.4.2 observable

```
observable = sym.empty("")
```

Default: sym.empty("")

Definition at line 36 of file SBMLode.m.

9.19.4.3 observable_name

```
observable_name = sym.empty("")
```

Default: sym.empty("")

Definition at line 44 of file SBMLode.m.

9.19.4.4 param

```
param = sym.empty("")
```

Default: sym.empty("")

Definition at line 52 of file SBMLode.m.

9.19.4.5 parameter

```
parameter = sym.empty("")
```

Default: sym.empty("")

Definition at line 60 of file SBMLode.m.

9.19.4.6 constant

```
constant = sym.empty("")
```

Default: sym.empty("")

Definition at line 68 of file SBMLode.m.

9.19.4.7 reaction

```
reaction = sym.empty("")
```

Default: sym.empty("")

Definition at line 76 of file SBMLode.m.

9.19.4.8 compartment

```
compartment = sym.empty("")
```

Default: sym.empty("")

Definition at line 84 of file SBMLode.m.

9.19.4.9 volume

```
volume = sym.empty("")
```

Default: sym.empty("")

Definition at line 92 of file SBMLode.m.

9.19.4.10 kvolume

```
kvolume = sym.empty("")
```

Default: sym.empty("")

Definition at line 100 of file SBMLode.m.

9.19.4.11 initState

```
initState = sym.empty("")
```

Default: sym.empty("")

Definition at line 108 of file SBMLode.m.

9.19.4.12 condition

```
condition = sym.empty("")
```

Default: sym.empty("")

Definition at line 116 of file SBMLode.m.

9.19.4.13 flux

```
flux = sym.empty("")
```

Default: sym.empty("")

Definition at line 124 of file SBMLode.m.

9.19.4.14 stochiometry

```
stochiometry = sym.empty("")
```

Default: sym.empty("")

Definition at line 132 of file SBMLode.m.

9.19.4.15 xdot

```
xdot = sym.empty("")
```

Default: sym.empty("")

Definition at line 140 of file SBMLode.m.

9.19.4.16 trigger

```
trigger = sym.empty("")
```

Default: sym.empty("")

Definition at line 148 of file SBMLode.m.

9.19.4.17 bolus

```
bolus = sym.empty("")
```

Default: sym.empty("")

Definition at line 156 of file SBMLode.m.

9.19.4.18 funmath

```
funmath = cell.empty("")
```

Default: cell.empty("")

Definition at line 164 of file SBMLode.m.

9.19.4.19 time_symbol

```
time_symbol = char.empty("")
```

Default: char.empty("")

Definition at line 174 of file SBMLode.m.

9.19.4.20 pnom

```
pnom = double.empty("")
```

Default: double.empty("")

Definition at line 182 of file SBMLode.m.

9.19.4.21 knom

```
knom = double.empty("")
```

Default: double.empty("")

Definition at line 190 of file SBMLode.m.

9.20 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>
```

Static Public Member Functions

- static int workSteadyStateProblem (UserData *udata, TempData *tdata, ReturnData *rdata, int it, Solver *solver, Model *model)
- static int applyNewtonsMethod (UserData *udata, ReturnData *rdata, TempData *tdata, int newton_try, Model *model, NewtonSolver *newtonSolver)
- static int getNewtonOutput (TempData *tdata, ReturnData *rdata, int newton_status, double run_time, int nx)
- static int getNewtonSimulation (UserData *udata, TempData *tdata, ReturnData *rdata, Solver *solver, Model *model)
- static int linsolveSPBCG (UserData *udata, ReturnData *rdata, TempData *tdata, int ntry, int nnewt, N_Vector ns_delta, Model *model)

9.20.1 Detailed Description

Definition at line 21 of file steadystateproblem.h.

9.20.2 Member Function Documentation

9.20.2.1 workSteadyStateProblem()

```
int workSteadyStateProblem (
            UserData * udata,
            TempData * tdata,
            ReturnData * rdata,
            int it,
            Solver * solver,
            Model * model )  [static]
```

```
tries to determine the steady state of the ODE system by a Newton
```

solver uses forward intergration, if the Newton solver fails

Parameters

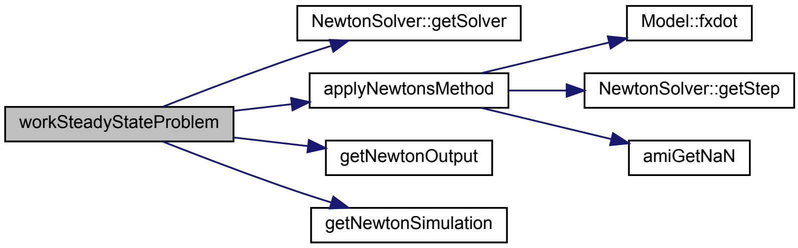
in	*udata*	pointer to the user data struct **Type**: UserData
in	*tdata*	pointer to the temporary data struct **Type**: UserData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
out	*rdata*	pointer to the return data struct **Type**: ReturnData

Returns

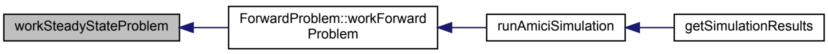
status flag indicating success of execution
Type: int

Definition at line 16 of file steadystateproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.20.2.2 applyNewtonsMethod()

```
int applyNewtonsMethod (
            UserData * udata,
            ReturnData * rdata,
            TempData * tdata,
            int newton_try,
            Model * model,
            NewtonSolver * newtonSolver )  [static]
```

applyNewtonsMethod applies Newtons method to the current state x to find the steady state

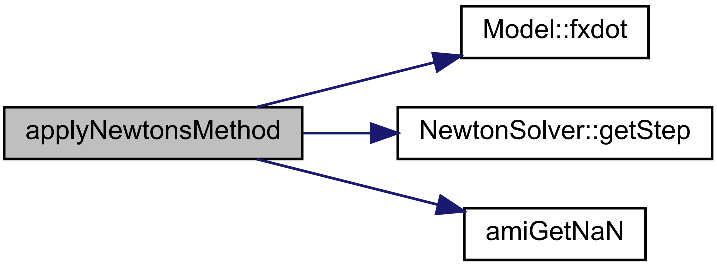
```
applyNewtonsMethod applies Newtons method to the current state x to
```

find the steady state

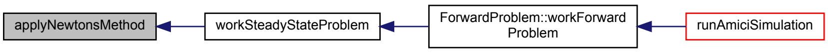
```
@param[in] udata pointer to the user data struct <br><b>Type</b>: UserData
@param[in] tdata pointer to the temporary data struct <br><b>Type</b>: TempData
@param[out] tdata pointer to the temporary data struct <br><b>Type</b>: TempData
@param[out] rdata pointer to the return data struct <br><b>Type</b>: ReturnData
@param[in] newton_try integer for the try number of the Newton solver
@return status flag indicating success of execution <br><b>Type</b>: int
```

Definition at line 84 of file steadystateproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.20.2.3 getNewtonOutput()

```
int getNewtonOutput (
            TempData * tdata,
            ReturnData * rdata,
            int newton_status,
            double run_time,
            int nx )  [static]
```

```
getNewtonOutput stores the output of the Newton solver run.

@param[in] udata pointer to the user data struct <br><b>Type</b>: UserData
@param[in] tdata pointer to the temporary data struct <br><b>Type</b>: TempData
@param[out] rdata pointer to the return data struct <br><b>Type</b>: ReturnData
@param[in] newton_status integer flag indicating the run of the
```

Newton solver

Parameters

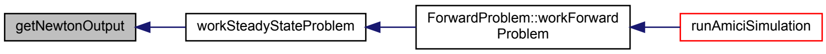
in	*run_time*	double computation time of the Newton solver

Returns

status flag indicating success of execution
Type: int

Definition at line 238 of file steadystateproblem.cpp.

Here is the caller graph for this function:



9.20.2.4 getNewtonSimulation()

```
int getNewtonSimulation (
            UserData * udata,
            TempData * tdata,
            ReturnData * rdata,
            Solver * solver,
            Model * model ) [static]
```

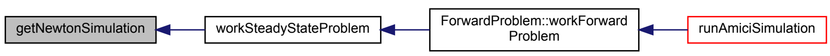
`getNewtonSimulation solves the forward problem, if the first Newton`

solver run did not succeed.

```
@param[in] udata pointer to the user data struct <br><b>Type</b>: UserData
@param[in] tdata pointer to the temporary data struct <br><b>Type</b>: TempData
@param[in] rdata pointer to the return data struct <br><b>Type</b>: ReturnData
@param[out] rdata pointer to the return data struct <br><b>Type</b>: ReturnData
@return status flag indicating success of execution <br><b>Type</b>: int
```

Definition at line 280 of file steadystateproblem.cpp.

Here is the caller graph for this function:



9.20.2.5 linsolveSPBCG()

```
int linsolveSPBCG (
            UserData * udata,
            ReturnData * rdata,
            TempData * tdata,
            int ntry,
            int nnewt,
            N_Vector ns_delta,
            Model * model ) [static]
```

`linsolveSPBCG solves the linear system for the Newton iteration by`

using the BiCGStab algorithm. This routines is to be stored in another file in near future.

Parameters

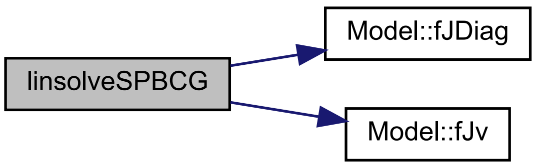
in	*udata*	pointer to the user data struct **Type**: UserData
out	*rdata*	pointer to the return data struct **Type**: ReturnData
in	*tdata*	pointer to the temporary data struct **Type**: TempData
out	*tdata*	pointer to the temporary data struct **Type**: TempData
in	*ami_mem*	pointer to the solver memory block **Type**: $*$void
in	*ntry*	intger number of Newton solver try
in	*nnewt*	intger number of Newton steps in the current Newton solver try
out	*delta*	N_Vector solution of the linear system

Returns

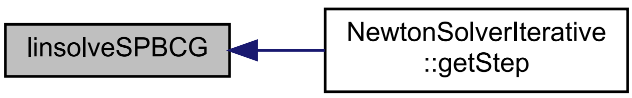
status flag indicating success of execution
Type: int

Definition at line 347 of file steadystateproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

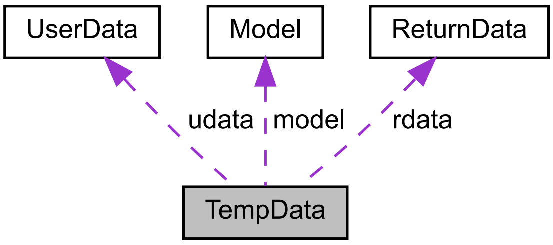


9.21 TempData Class Reference

struct that provides temporary storage for different variables

`#include <tdata.h>`

Collaboration diagram for TempData:



Public Member Functions

- TempData (const UserData *udata, Model *model, ReturnData *rdata)

    Default constructor.

Public Attributes

- realtype * p = nullptr
- realtype t
- N_Vector x
- N_Vector x_old
- N_Vector * x_disc
- N_Vector * xdot_disc
- N_Vector * xdot_old_disc
- N_Vector dx
- N_Vector dx_old
- N_Vector xdot
- N_Vector xdot_old
- N_Vector xB
- N_Vector xB_old
- N_Vector dxB
- N_Vector xQB
- N_Vector xQB_old
- N_Vector * sx
- N_Vector * sdx
- DlsMat Jtmp
- realtype * llhS0
- realtype * Jy
- realtype * dJydp
- realtype * dJydy

- realtype ∗ dJydsigma
- realtype ∗ dJydx
- realtype ∗ Jz
- realtype ∗ dJzdp
- realtype ∗ dJzdx
- realtype ∗ dJzdz
- realtype ∗ dJzdsigma
- realtype ∗ dJrzdz
- realtype ∗ dJrzdsigma
- realtype ∗ dzdx
- realtype ∗ dzdp
- realtype ∗ drzdx
- realtype ∗ drzdp
- realtype ∗ dydp
- realtype ∗ dydx
- realtype ∗ yS0
- realtype ∗ sigmay
- realtype ∗ dsigmaydp
- realtype ∗ sigmaz
- realtype ∗ dsigmazdp
- int ∗ rootsfound
- int ∗ rootidx
- int ∗ nroots
- realtype ∗ rootvals
- realtype ∗ h
- realtype ∗ h_udata
- realtype ∗ deltax
- realtype ∗ deltasx
- realtype ∗ deltaxB
- realtype ∗ deltaqB
- int which
- realtype ∗ discs
- realtype ∗ irdiscs
- SlsMat J = NULL
- realtype ∗ dxdotdp = NULL
- realtype ∗ w = NULL
- realtype ∗ dwdx = NULL
- realtype ∗ dwdp = NULL
- realtype ∗ M = NULL
- realtype ∗ dfdx = NULL
- realtype ∗ stau = NULL
- int nplist
- int iroot = 0
- booleantype nan_dxdotdp = false
- booleantype nan_J = false
- booleantype nan_JDiag = false
- booleantype nan_JSparse = false
- booleantype nan_xdot = false
- booleantype nan_xBdot = false
- booleantype nan_qBdot = false
- const UserData ∗ udata
- Model ∗ model
- ReturnData ∗ rdata
- Solver ∗ solver = nullptr

9.21.1 Detailed Description

Definition at line 17 of file tdata.h.

9.21.2 Constructor & Destructor Documentation

9.21.2.1 TempData()

```
TempData (
            const UserData * udata,
            Model * model,
            ReturnData * rdata )
```

Parameters

in	*udata*	pointer to the user data struct **Type**: UserData
in	*model*	pointer to model specification object **Type**: Model
in	*rdata*	pointer to the return data struct **Type**: ReturnData

Definition at line 8 of file tdata.cpp.

Here is the call graph for this function:

9.21.3 Member Data Documentation

9.21.3.1 p

```
realtype* p = nullptr
```

parameter array, unscaled

Definition at line 32 of file tdata.h.

9.21.3.2 t

```
realtype t
```

current time

Definition at line 35 of file tdata.h.

9.21.3.3 x

```
N_Vector x
```

state vector

Definition at line 38 of file tdata.h.

9.21.3.4 x_old

```
N_Vector x_old
```

old state vector

Definition at line 40 of file tdata.h.

9.21.3.5 x_disc

```
N_Vector* x_disc
```

array of state vectors at discontinuities

Definition at line 42 of file tdata.h.

9.21.3.6 xdot_disc

```
N_Vector* xdot_disc
```

array of differential state vectors at discontinuities

Definition at line 44 of file tdata.h.

9.21.3.7 xdot_old_disc

```
N_Vector* xdot_old_disc
```

array of old differential state vectors at discontinuities

Definition at line 46 of file tdata.h.

9.21.3.8 dx

```
N_Vector dx
```

differential state vector

Definition at line 48 of file tdata.h.

9.21.3.9 dx_old

```
N_Vector dx_old
```

old differential state vector

Definition at line 50 of file tdata.h.

9.21.3.10 xdot

```
N_Vector xdot
```

time derivative state vector

Definition at line 52 of file tdata.h.

9.21.3.11 xdot_old

```
N_Vector xdot_old
```

old time derivative state vector

Definition at line 54 of file tdata.h.

9.21.3.12 xB

```
N_Vector xB
```

adjoint state vector

Definition at line 56 of file tdata.h.

9.21.3.13 xB_old

```
N_Vector xB_old
```

old adjoint state vector

Definition at line 58 of file tdata.h.

9.21.3.14 dxB

```
N_Vector dxB
```

differential adjoint state vector

Definition at line 60 of file tdata.h.

9.21.3.15 xQB

```
N_Vector xQB
```

quadrature state vector

Definition at line 62 of file tdata.h.

9.21.3.16 xQB_old

```
N_Vector xQB_old
```

old quadrature state vector

Definition at line 64 of file tdata.h.

9.21.3.17 sx

```
N_Vector* sx
```

sensitivity state vector array

Definition at line 66 of file tdata.h.

9.21.3.18 sdx

```
N_Vector* sdx
```

differential sensitivity state vector array

Definition at line 68 of file tdata.h.

9.21.3.19 Jtmp

```
DlsMat Jtmp
```

Jacobian

Definition at line 70 of file tdata.h.

9.21.3.20 llhS0

```
realtype* llhS0
```

parameter derivative of likelihood array

Definition at line 73 of file tdata.h.

9.21.3.21 Jy

```
realtype* Jy
```

data likelihood

Definition at line 75 of file tdata.h.

9.21.3.22 dJydp

```
realtype* dJydp
```

parameter derivative of data likelihood

Definition at line 77 of file tdata.h.

9.21.3.23 dJydy

```
realtype* dJydy
```

observable derivative of data likelihood

Definition at line 79 of file tdata.h.

9.21.3.24 dJydsigma

```
realtype* dJydsigma
```

observable sigma derivative of data likelihood

Definition at line 81 of file tdata.h.

9.21.3.25 dJydx

```
realtype* dJydx
```

state derivative of data likelihood

Definition at line 83 of file tdata.h.

9.21.3.26 Jz

```
realtype* Jz
```

event likelihood

Definition at line 85 of file tdata.h.

9.21.3.27 dJzdp

```
realtype* dJzdp
```

parameter derivative of event likelihood

Definition at line 87 of file tdata.h.

9.21.3.28 dJzdx

```
realtype* dJzdx
```

state derivative of event likelihood

Definition at line 89 of file tdata.h.

9.21.3.29 dJzdz

```
realtype* dJzdz
```

event ouput derivative of event likelihood

Definition at line 91 of file tdata.h.

9.21.3.30 dJzdsigma

```
realtype* dJzdsigma
```

event sigma derivative of event likelihood

Definition at line 93 of file tdata.h.

9.21.3.31 dJrzdz

```
realtype* dJrzdz
```

event ouput derivative of event likelihood at final timepoint

Definition at line 95 of file tdata.h.

9.21.3.32 dJrzdsigma

```
realtype* dJrzdsigma
```

event sigma derivative of event likelihood at final timepoint

Definition at line 97 of file tdata.h.

9.21.3.33 dzdx

```
realtype* dzdx
```

state derivative of event output

Definition at line 99 of file tdata.h.

9.21.3.34 dzdp

```
realtype* dzdp
```

parameter derivative of event output

Definition at line 101 of file tdata.h.

9.21.3.35 drzdx

```
realtype* drzdx
```

state derivative of event timepoint

Definition at line 103 of file tdata.h.

9.21.3.36 drzdp

```
realtype* drzdp
```

parameter derivative of event timepoint

Definition at line 105 of file tdata.h.

9.21.3.37 dydp

```
realtype* dydp
```

parameter derivative of observable

Definition at line 107 of file tdata.h.

9.21.3.38 dydx

```
realtype* dydx
```

state derivative of observable

Definition at line 109 of file tdata.h.

9.21.3.39 yS0

```
realtype* yS0
```

initial sensitivity of observable

Definition at line 111 of file tdata.h.

9.21.3.40 sigmay

```
realtype* sigmay
```

data standard deviation

Definition at line 113 of file tdata.h.

9.21.3.41 dsigmaydp

```
realtype* dsigmaydp
```

parameter derivative of data standard deviation

Definition at line 115 of file tdata.h.

9.21.3.42 sigmaz

```
realtype* sigmaz
```

event standard deviation

Definition at line 117 of file tdata.h.

9.21.3.43 dsigmazdp

```
realtype* dsigmazdp
```

parameter derivative of event standard deviation

Definition at line 119 of file tdata.h.

9.21.3.44 rootsfound

```
int* rootsfound
```

array of flags indicating which root has beend found

array of length nr with the indices of the user functions gi found to have a root. For i = 0, . . . ,nr 1 if gi has a root, and = 0 if not.

Definition at line 126 of file tdata.h.

9.21.3.45 rootidx

```
int* rootidx
```

array of index which root has been found

Definition at line 128 of file tdata.h.

9.21.3.46 nroots

```
int* nroots
```

array of number of found roots for a certain event type

Definition at line 130 of file tdata.h.

9.21.3.47 rootvals

```
realtype* rootvals
```

array of values of the root function

Definition at line 132 of file tdata.h.

9.21.3.48 h

```
realtype* h
```

temporary rootval storage to check crossing in secondary event

Definition at line 134 of file tdata.h.

9.21.3.49 h_udata

```
realtype* h_udata
```

flag indicating whether a certain heaviside function should be active or not Moved from UserData to TempData; TODO: better naming

Definition at line 139 of file tdata.h.

9.21.3.50 deltax

```
realtype* deltax
```

change in x

Definition at line 142 of file tdata.h.

9.21.3.51 deltasx

```
realtype* deltasx
```

change in sx

Definition at line 144 of file tdata.h.

9.21.3.52 deltaxB

```
realtype* deltaxB
```

change in xB

Definition at line 146 of file tdata.h.

9.21.3.53 deltaqB

```
realtype* deltaqB
```

change in qB

Definition at line 148 of file tdata.h.

9.21.3.54 which

```
int which
```

integer for indexing of backwards problems

Definition at line 151 of file tdata.h.

9.21.3.55 discs

```
realtype* discs
```

array containing the time-points of discontinuities

Definition at line 154 of file tdata.h.

9.21.3.56 irdiscs

```
realtype* irdiscs
```

array containing the index of discontinuities

Definition at line 156 of file tdata.h.

9.21.3.57 J

```
SlsMat J = NULL
```

tempory storage of Jacobian data across functions

Definition at line 159 of file tdata.h.

9.21.3.58 dxdotdp

```
realtype* dxdotdp = NULL
```

tempory storage of dxdotdp data across functions

Definition at line 161 of file tdata.h.

9.21.3.59 w

```
realtype* w = NULL
```

tempory storage of w data across functions

Definition at line 163 of file tdata.h.

9.21.3.60 dwdx

```
realtype* dwdx = NULL
```

tempory storage of dwdx data across functions

Definition at line 165 of file tdata.h.

9.21.3.61 dwdp

```
realtype* dwdp = NULL
```

tempory storage of dwdp data across functions

Definition at line 167 of file tdata.h.

9.21.3.62 M

```
realtype* M = NULL
```

tempory storage of M data across functions

Definition at line 169 of file tdata.h.

9.21.3.63 dfdx

```
realtype* dfdx = NULL
```

tempory storage of dfdx data across functions

Definition at line 171 of file tdata.h.

9.21.3.64 stau

```
realtype* stau = NULL
```

tempory storage of stau data across functions

Definition at line 173 of file tdata.h.

9.21.3.65 nplist

```
int nplist
```

number of parameters, copied from udata, necessary for deallocation

Definition at line 176 of file tdata.h.

9.21.3.66 iroot

```
int iroot = 0
```

current root index, will be increased during the forward solve and decreased during backward solve

Definition at line 180 of file tdata.h.

9.21.3.67 nan_dxdotdp

```
booleantype nan_dxdotdp = false
```

flag indicating whether a NaN in dxdotdp has been reported

Definition at line 183 of file tdata.h.

9.21.3.68 nan_J

```
booleantype nan_J = false
```

flag indicating whether a NaN in J has been reported

Definition at line 185 of file tdata.h.

9.21.3.69 nan_JDiag

```
booleantype nan_JDiag = false
```

flag indicating whether a NaN in JDiag has been reported

Definition at line 187 of file tdata.h.

9.21.3.70 nan_JSparse

```
booleantype nan_JSparse = false
```

flag indicating whether a NaN in JSparse has been reported

Definition at line 189 of file tdata.h.

9.21.3.71 nan_xdot

```
booleantype nan_xdot = false
```

flag indicating whether a NaN in xdot has been reported

Definition at line 191 of file tdata.h.

9.21.3.72 nan_xBdot

```
booleantype nan_xBdot = false
```

flag indicating whether a NaN in xBdot has been reported

Definition at line 193 of file tdata.h.

9.21.3.73 nan_qBdot

```
booleantype nan_qBdot = false
```

flag indicating whether a NaN in qBdot has been reported

Definition at line 195 of file tdata.h.

9.21.3.74 udata

```
const UserData* udata
```

attached UserData object

Definition at line 198 of file tdata.h.

9.21.3.75 model

```
Model* model
```

attached Model object

Definition at line 200 of file tdata.h.

9.21.3.76 rdata

```
ReturnData* rdata
```

attached ReturnData object

Definition at line 202 of file tdata.h.

9.21.3.77 solver

```
Solver* solver = nullptr
```

attached Solver object

Definition at line 204 of file tdata.h.

9.22 UserData Class Reference

struct that stores all user provided data

`#include <udata.h>`

Public Member Functions

- UserData ()

  Default constructor for testing and serialization.
- int unscaleParameters (const Model ∗model, double ∗bufferUnscaled) const

  unscales parameters according to the defined parameter scaling
- void print ()

Public Attributes

- int nmaxevent
- double ∗ qpositivex
- int ∗ plist
- int nplist
- int nt
- double ∗ p
- double ∗ k
- AMICI_parameter_scaling pscale
- double tstart
- double ∗ ts
- double ∗ pbar
- double ∗ xbar
- AMICI_sensi_order sensi
- double atol
- double rtol
- int maxsteps
- int newton_maxsteps
- int newton_maxlinsteps
- int newton_preeq
- int newton_precon
- int ism
- AMICI_sensi_meth sensi_meth
- int linsol
- int interpType
- int lmm
- int iter
- booleantype stldet
- double ∗ x0data
- double ∗ sx0data
- int ordering

Protected Member Functions

- void init ()

9.22.1 Detailed Description

Definition at line 10 of file udata.h.

9.22.2 Member Function Documentation

9.22.2.1 unscaleParameters()

```
int unscaleParameters (
            const Model * model,
            double * bufferUnscaled ) const
```

Parameters

in	*model*	pointer to model specification object **Type**: Model
out	*bufferUnscaled*	unscaled parameters are written to the array **Type**: double

unscaleParameters removes parameter scaling according to the parameter scaling in pscale

Parameters

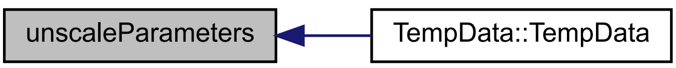
in	*model*	pointer to model specification object **Type**: Model
out	*bufferUnscaled*	unscaled parameters are written to the array **Type**: double

Returns

status flag indicating success of execution
Type: int

Definition at line 8 of file udata.cpp.

Here is the caller graph for this function:



9.22.2.2 print()

```
void print ( )
```

function to print the contents of the UserData object

Definition at line 92 of file udata.cpp.

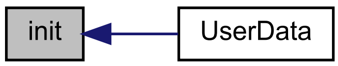
9.22.2.3 init()

```
void init ( ) [protected]
```

function to initialize the contents of the UserData object

Definition at line 58 of file udata.cpp.

Here is the caller graph for this function:



9.22.3 Member Data Documentation

9.22.3.1 nmaxevent

```
int nmaxevent
```

maximal number of events to track

Definition at line 31 of file udata.h.

9.22.3.2 qpositivex

```
double* qpositivex
```

positivity flag

Definition at line 34 of file udata.h.

9.22.3.3 plist

```
int* plist
```

parameter selection and reordering

Definition at line 37 of file udata.h.

9.22.3.4 nplist

```
int nplist
```

number of parameters in plist

Definition at line 39 of file udata.h.

9.22.3.5 nt

```
int nt
```

number of timepoints

Definition at line 42 of file udata.h.

9.22.3.6 p

```
double* p
```

parameter array

Definition at line 45 of file udata.h.

9.22.3.7 k

```
double* k
```

constants array

Definition at line 48 of file udata.h.

9.22.3.8 pscale

```
AMICI_parameter_scaling pscale
```

parameter transformation of p

Definition at line 51 of file udata.h.

9.22.3.9 tstart

```
double tstart
```

starting time

Definition at line 54 of file udata.h.

9.22.3.10 ts

```
double* ts
```

timepoints

Definition at line 56 of file udata.h.

9.22.3.11 pbar

```
double* pbar
```

scaling of parameters

Definition at line 59 of file udata.h.

9.22.3.12 xbar

```
double* xbar
```

scaling of states

Definition at line 61 of file udata.h.

9.22.3.13 sensi

```
AMICI_sensi_order sensi
```

flag indicating whether sensitivities are supposed to be computed

Definition at line 64 of file udata.h.

9.22.3.14 atol

```
double atol
```

absolute tolerances for integration

Definition at line 66 of file udata.h.

9.22.3.15 rtol

```
double rtol
```

relative tolerances for integration

Definition at line 68 of file udata.h.

9.22.3.16 maxsteps

```
int maxsteps
```

maximum number of allowed integration steps

Definition at line 70 of file udata.h.

9.22.3.17 newton_maxsteps

```
int newton_maxsteps
```

maximum number of allowed Newton steps for steady state computation

Definition at line 73 of file udata.h.

9.22.3.18 newton_maxlinsteps

```
int newton_maxlinsteps
```

maximum number of allowed linear steps per Newton step for steady state computation

Definition at line 76 of file udata.h.

9.22.3.19 newton_preeq

```
int newton_preeq
```

Preequilibration of model via NEwton solver?

Definition at line 78 of file udata.h.

9.22.3.20 newton_precon

```
int newton_precon
```

Which preconditioner is to be used in the case of iterative linear Newton solvers

Definition at line 81 of file udata.h.

9.22.3.21 ism

```
int ism
```

internal sensitivity method

a flag used to select the sensitivity solution method. Its value can be CV SIMULTANEOUS or CV STAGGERED. Only applies for Forward Sensitivities.

Definition at line 88 of file udata.h.

9.22.3.22 sensi_meth

```
AMICI_sensi_meth sensi_meth
```

method for sensitivity computation

Definition at line 91 of file udata.h.

9.22.3.23 linsol

```
int linsol
```

linear solver specification

Definition at line 94 of file udata.h.

9.22.3.24 interpType

```
int interpType
```

interpolation type

specifies the interpolation type for the forward problem solution which is then used for the backwards problem. can be either CV_POLYNOMIAL or CV_HERMITE

Definition at line 102 of file udata.h.

9.22.3.25 lmm

```
int lmm
```

linear multistep method

specifies the linear multistep method and may be one of two possible values: CV ADAMS or CV BDF.

Definition at line 109 of file udata.h.

9.22.3.26 iter

```
int iter
```

nonlinear solver

specifies the type of nonlinear solver iteration and may be either CV NEWTON or CV FUNCTIONAL.

Definition at line 116 of file udata.h.

9.22.3.27 stldet

```
booleantype stldet
```

flag controlling stability limit detection

Definition at line 119 of file udata.h.

9.22.3.28 x0data

```
double* x0data
```

state initialisation

Definition at line 122 of file udata.h.

9.22.3.29 sx0data

```
double* sx0data
```

sensitivity initialisation

Definition at line 125 of file udata.h.

9.22.3.30 ordering

```
int ordering
```

state ordering

Definition at line 128 of file udata.h.

10 File Documentation

10.1 amiwrap.m File Reference

AMIWRAP generates c++ mex files for the simulation of systems of differential equations via CVODES and IDAS.

Functions

- noret::substitute amiwrap (matlabtypesubstitute varargin)
  AMIWRAP generates c++ mex files for the simulation of systems of differential equations via CVODES and IDAS.

10.1.1 Function Documentation

10.1.1.1 amiwrap()

```
noret::substitute amiwrap (
            matlabtypesubstitute varargin )
```

Parameters

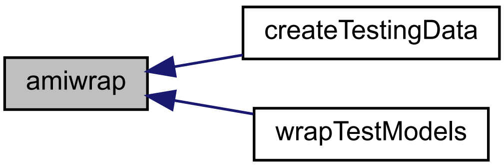
varargin	`amiwrap ( modelname, symfun, tdir, o2flag )` *Required Parameters for varargin:* • modelname specifies the name of the model which will be later used for the naming of the simulation file • symfun specifies a function which executes model definition see Model Definition for details • tdir target directory where the simulation file should be placed **Default:** $AMICIDIR/models/modelname • o2flag boolean whether second order sensitivities should be enabled **Default:** false

Return values

o2flag	void

Definition at line 17 of file amiwrap.m.

Here is the caller graph for this function:



10.2 SBML2AMICI.m File Reference

SBML2AMICI generates AMICI model definition files from SBML.

Functions

- noret::substitute SBML2AMICI (matlabtypesubstitute filename, matlabtypesubstitute modelname)
  SBML2AMICI generates AMICI model definition files from SBML.

10.2.1 Function Documentation

10.2.1.1 SBML2AMICI()

```
noret::substitute SBML2AMICI (
            matlabtypesubstitute filename,
            matlabtypesubstitute modelname )
```

Parameters

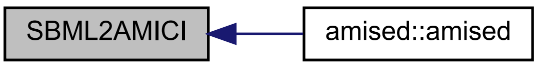
filename	name of the SBML file (withouth extension)
modelname	name of the model, this will define the name of the output file (default: input filename)

Return values

modelname	void

Definition at line 17 of file SBML2AMICI.m.

Here is the caller graph for this function:



10.3 SBMLimporter/computeBracketLevel.m File Reference

Compute the bracket level for the input string cstr. The bracket level is computed for every char in cstr and indicates how many brackets have been opened up to this point. The bracket level is useful to parse the arguments of functions in cstr. For this purpose functions will have the same bracket level as the opening bracket of the corresponding function call.

Functions

- mlhsInnerSubst<::∗int > computeBracketLevel (::∗char cstr)

  Compute the bracket level for the input string cstr. The bracket level is computed for every char in cstr and indicates how many brackets have been opened up to this point. The bracket level is useful to parse the arguments of functions in cstr. For this purpose functions will have the same bracket level as the opening bracket of the corresponding function call.

10.3.1 Function Documentation

10.3.1.1 computeBracketLevel()

```
mlhsInnerSubst<::*int > computeBracketLevel (
            ::*char cstr )
```

Parameters

cstr	input string

Return values

brl	bracket levels

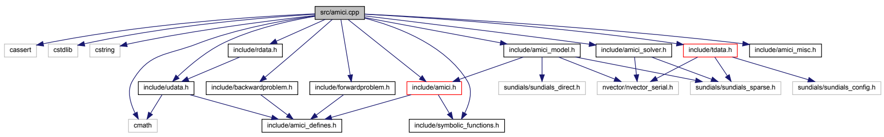
Definition at line 17 of file computeBracketLevel.m.

10.4 src/amici.cpp File Reference

core routines for integration

```
#include <cassert>
#include <cstdlib>
#include <cstring>
#include <cmath>
#include "include/amici_model.h"
#include "include/amici_solver.h"
#include "include/backwardproblem.h"
#include "include/forwardproblem.h"
#include "include/rdata.h"
#include "include/tdata.h"
#include "include/udata.h"
#include <include/amici.h>
#include <include/amici_misc.h>
#include <include/symbolic_functions.h>
```

Include dependency graph for amici.cpp:



Macros

- #define **_USE_MATH_DEFINES** /∗ MS definition of PI and other constants ∗/
- #define **M_PI** 3.14159265358979323846

Functions

- int runAmiciSimulation (UserData ∗udata, const ExpData ∗edata, ReturnData ∗rdata, Model ∗model)
- void printErrMsgIdAndTxt (const char ∗identifier, const char ∗msg,...)
- void printWarnMsgIdAndTxt (const char ∗identifier, const char ∗msg,...)

Variables

- msgIdAndTxtFp **errMsgIdAndTxt** = &printErrMsgIdAndTxt
- msgIdAndTxtFp **warnMsgIdAndTxt** = &printWarnMsgIdAndTxt

10.4.1 Function Documentation

10.4.1.1 runAmiciSimulation()

```
int runAmiciSimulation (
            UserData * udata,
            const ExpData * edata,
            ReturnData * rdata,
            Model * model )
```

runAmiciSimulation is the core integration routine. It initializes the solver and temporary storage in tdata and runs the forward and backward problem.

Parameters

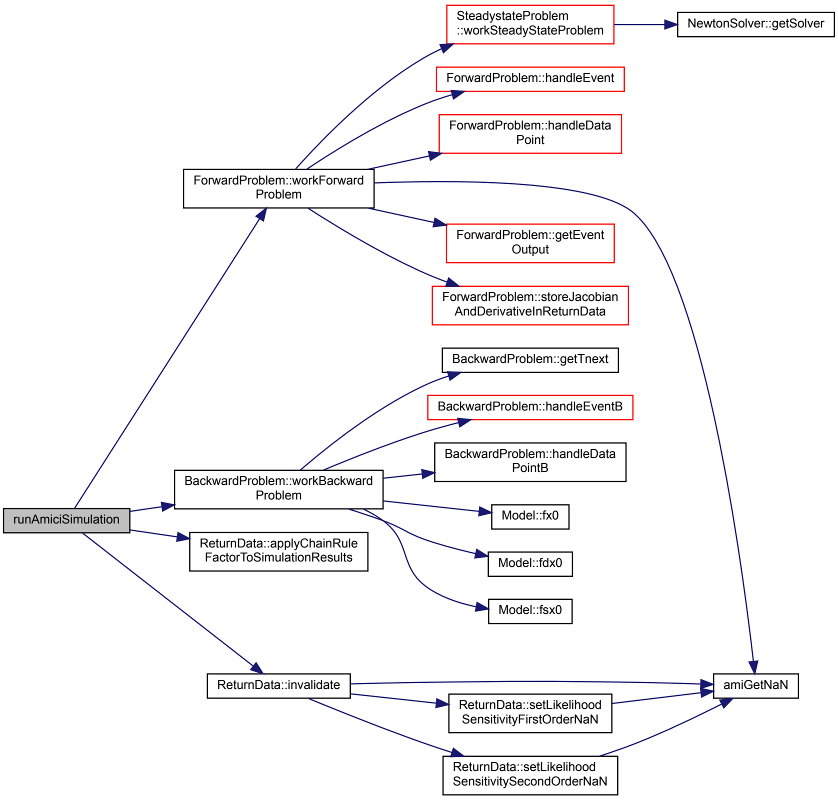
in	*udata*	pointer to user data object **Type**: UserData
in	*edata*	pointer to experimental data object **Type**: ExpData
in	*rdata*	pointer to return data object **Type**: ReturnData
in	*model*	pointer to model specification object **Type**: Model

Returns

status status flag indicating (un)successful execution
Type: int

Definition at line 39 of file amici.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

10.4.1.2 printErrMsgIdAndTxt()

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

printErrMsgIdAndTxt prints a specified error message associated to the specified identifier

Parameters

in	*identifier*	error identifier **Type**: char
in	*msg*	error message **Type**: char

Returns

void

Definition at line 77 of file amici.cpp.

10.4.1.3 printWarnMsgIdAndTxt()

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

printErrMsgIdAndTxt prints a specified warning message associated to the specified identifier

Parameters

in	*identifier*	warning identifier **Type**: char
in	*msg*	warning message **Type**: char

Returns

void

Definition at line 88 of file amici.cpp.

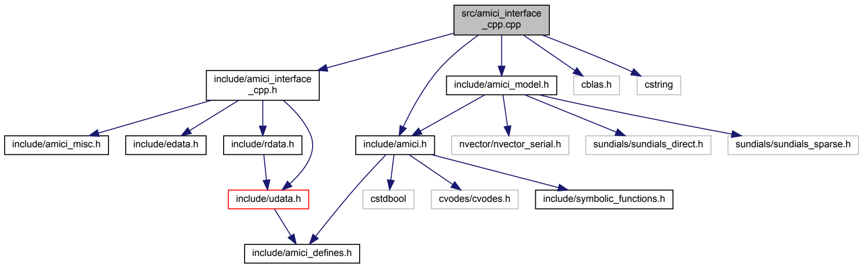
10.5 src/amici_interface_cpp.cpp File Reference

core routines for cpp interface

```
#include "include/amici_interface_cpp.h"
#include "include/amici.h"
#include <include/amici_model.h>
#include <cblas.h>
```

`#include <cstring>`

Include dependency graph for amici_interface_cpp.cpp:



Functions

- ReturnData ∗ getSimulationResults (Model ∗model, UserData ∗udata, const ExpData ∗edata)
- void amici_dgemm (AMICI_BLAS_LAYOUT layout, AMICI_BLAS_TRANSPOSE TransA, AMICI_BLAS_TRANSPOSE 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 (AMICI_BLAS_LAYOUT layout, AMICI_BLAS_TRANSPOSE 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)

10.5.1 Function Documentation

10.5.1.1 getSimulationResults()

```
ReturnData* getSimulationResults (
            Model * model,
            UserData * udata,
            const ExpData * edata )
```

getSimulationResults is the core cpp interface function. It initializes the model and return data and then calls the core simulation routine.

Parameters

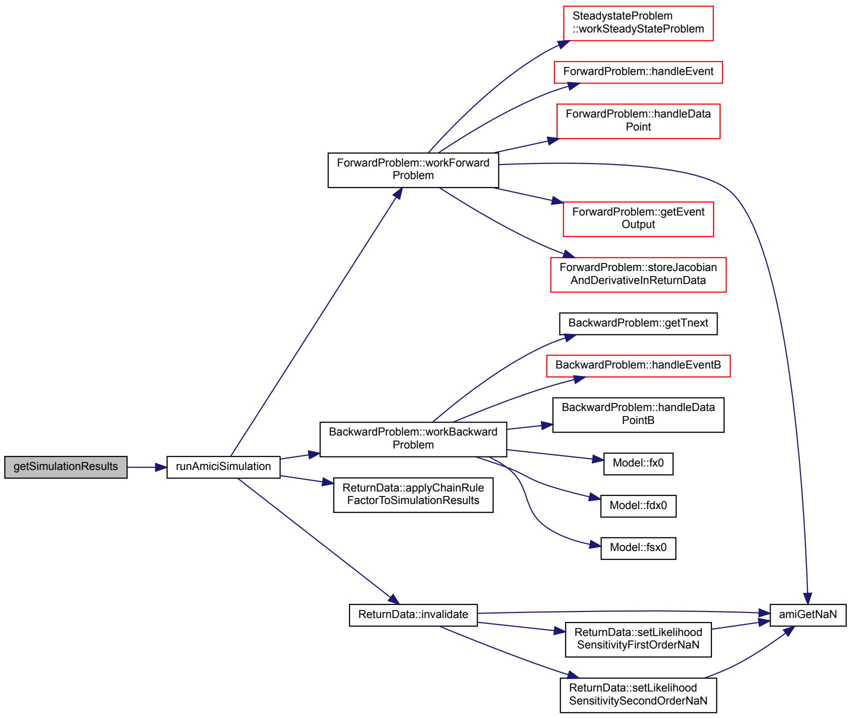
in	*model*	pointer to the model object, this is necessary to perform dimension checks **Type**: Model
in	*udata*	pointer to user data object **Type**: UserData
in	*edata*	pointer to experimental data object **Type**: ExpData

Returns

rdata pointer to return data object
Type: ReturnData

Definition at line 31 of file amici_interface_cpp.cpp.

Here is the call graph for this function:



10.5.1.2 amici_dgemm()

```
void amici_dgemm (
            AMICI_BLAS_LAYOUT layout,
            AMICI_BLAS_TRANSPOSE TransA,
            AMICI_BLAS_TRANSPOSE 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

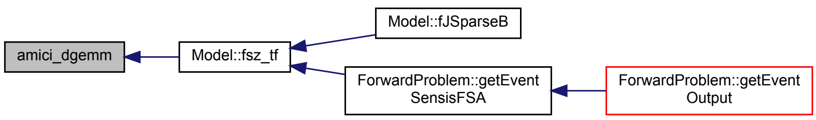
in	*layout*	can be AMICI_BLAS_ColMajor or AMICI_BLAS_RowMajor.

Parameters

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)

Definition at line 60 of file amici_interface_cpp.cpp.

Here is the caller graph for this function:



10.5.1.3 amici_dgemv()

```
void amici_dgemv (
            AMICI_BLAS_LAYOUT layout,
            AMICI_BLAS_TRANSPOSE 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

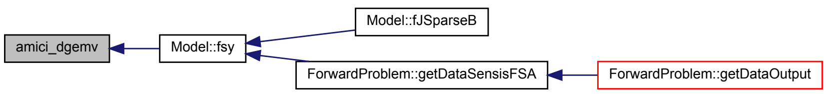
in	*layout*	can be AMICI_BLAS_ColMajor or AMICI_BLAS_RowMajor.

Parameters

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

Definition at line 83 of file amici_interface_cpp.cpp.

Here is the caller graph for this function:

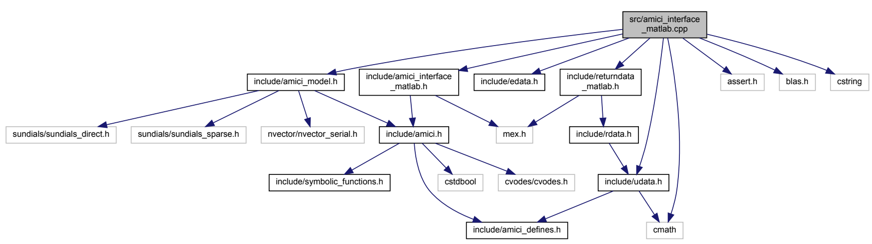


10.6 src/amici_interface_matlab.cpp File Reference

core routines for mex interface

```
#include "include/amici_interface_matlab.h"
#include "include/amici_model.h"
#include "include/edata.h"
#include "include/returndata_matlab.h"
#include "include/udata.h"
#include <assert.h>
#include <blas.h>
#include <cstring>
#include <cmath>
```

Include dependency graph for amici_interface_matlab.cpp:



Macros

- #define **_USE_MATH_DEFINES** /* MS definition of PI and other constants */
- #define **M_PI** 3.14159265358979323846
- #define readOptionScalar(OPTION, TYPE)
- #define readOptionData(OPTION)

Functions

- void mexFunction (int nlhs, mxArray *plhs[ ], int nrhs, const mxArray *prhs[ ])
- UserData * userDataFromMatlabCall (const mxArray *prhs[ ], int nrhs, Model *model)

  userDataFromMatlabCall extracts information from the matlab call and returns the corresponding UserData struct
- char amici_blasCBlasTransToBlasTrans (AMICI_BLAS_TRANSPOSE trans)
- void amici_dgemm (AMICI_BLAS_LAYOUT layout, AMICI_BLAS_TRANSPOSE TransA, AMICI_BLAS_TRANSPOSE 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 (AMICI_BLAS_LAYOUT layout, AMICI_BLAS_TRANSPOSE 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)
- ExpData * expDataFromMatlabCall (const mxArray *prhs[ ], const UserData *udata, Model *model)

10.6.1 Detailed Description

This file defines the fuction mexFunction which is executed upon calling the mex file from matlab

10.6.2 Macro Definition Documentation

10.6.2.1 readOptionScalar

```
#define readOptionScalar(
                OPTION,
                TYPE )
```

Value:

```
if (mxGetProperty(prhs[3], 0, #OPTION)) {                              \
        udata->OPTION = (TYPE)mxGetScalar(mxGetProperty(prhs[3], 0, #OPTION)); \
    } else {                                                                   \
        warnMsgIdAndTxt("AMICI:mex:OPTION",                                    \
                        "Provided options do not have field " #OPTION "!");    \
        goto freturn;                                                          \
    }
```

@ brief extract information from a property of a matlab class (scalar) @ param OPTION name of the property @ param TYPE class to which the information should be cast

Definition at line 30 of file amici_interface_matlab.cpp.

10.6.2.2 readOptionData

```
#define readOptionData(
              OPTION )
```

Value:

```
if (mxGetProperty(prhs[3], 0, #OPTION)) {                              \
        mxArray *a = mxGetProperty(prhs[3], 0, #OPTION);                   \
        int len = (int)mxGetM(a) * mxGetN(a);                              \
        udata->OPTION = new double[len];                                   \
        memcpy(udata->OPTION, mxGetData(a), sizeof(double) * len);         \
    } else {                                                               \
        warnMsgIdAndTxt("AMICI:mex:OPTION",                                \
                        "Provided options do not have field " #OPTION "!"); \
        goto freturn;                                                      \
    }
```

@ brief extract information from a property of a matlab class (matrix) @ param OPTION name of the property

Definition at line 43 of file amici_interface_matlab.cpp.

10.6.3 Function Documentation

10.6.3.1 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

in	*nlhs*	number of output arguments of the matlab call **Type**: int
out	*plhs*	pointer to the array of output arguments **Type**: mxArray
in	*nrhs*	number of input arguments of the matlab call **Type**: int
in	*prhs*	pointer to the array of input arguments **Type**: mxArray

Returns

void

Definition at line 65 of file amici_interface_matlab.cpp.

10.6.3.2 userDataFromMatlabCall()

```
UserData* userDataFromMatlabCall (
            const mxArray * prhs[],
            int nrhs,
            Model * model )
```

userDataFromMatlabCall parses the input from the matlab call and writes it to an UserData class object

Parameters

in	*nrhs*	number of input arguments of the matlab call **Type**: int
in	*prhs*	pointer to the array of input arguments **Type**: mxArray
in	*model*	pointer to the model object, this is necessary to perform dimension checks **Type**: Model

Returns

udata pointer to user data object
Type: UserData

Definition at line 116 of file amici_interface_matlab.cpp.

10.6.3.3 amici_blasCBlasTransToBlasTrans()

```
char amici_blasCBlasTransToBlasTrans (
            AMICI_BLAS_TRANSPOSE trans )
```

amici_blasCBlasTransToBlasTrans translates AMICI_BLAS_TRANSPOSE values to CBlas readable strings

Parameters

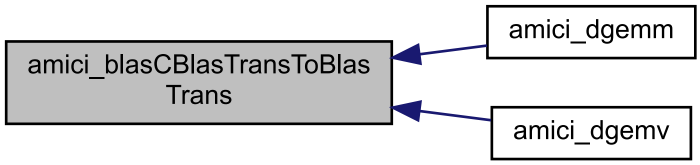
in	*trans*	flag indicating transposition and complex conjugation **Type**: AMICI_BLAS_TRANSPOSE

Returns

cblastrans CBlas readable CHAR indicating transposition and complex conjugation
Type: char

Definition at line 323 of file amici_interface_matlab.cpp.

Here is the caller graph for this function:



10.6.3.4 amici_dgemm()

```
void amici_dgemm (
            AMICI_BLAS_LAYOUT layout,
            AMICI_BLAS_TRANSPOSE TransA,
            AMICI_BLAS_TRANSPOSE 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 CBlas matrix matrix multiplication routine dgemm. This routines computes C = alpha∗A∗B + beta∗C with A: [MxK] B:[KxN] C:[MxN]

Parameters

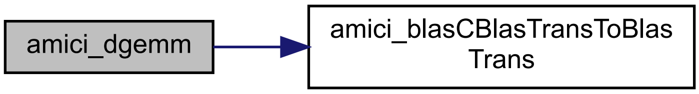
in	*layout*	always needs to be AMICI_BLAS_ColMajor.
in	*TransA*	flag indicating whether A should be transposed before multiplication
in	*TransB*	flag indicating whether B should be transposed before multiplication
in	*M*	number of rows in A/C
in	*N*	number of columns in B/C
in	*K*	number of rows in B, 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)

Returns

void

Definition at line 355 of file amici_interface_matlab.cpp.

Here is the call graph for this function:



10.6.3.5 amici_dgemv()

```
void amici_dgemv (
            AMICI_BLAS_LAYOUT layout,
            AMICI_BLAS_TRANSPOSE 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 CBlas matrix vector multiplication routine dgemv. This routines computes y = alpha∗A∗x + beta∗y with A: [MxN] x:[Nx1] y:[Mx1]

Parameters

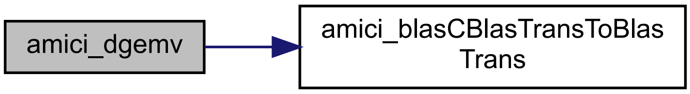
in	*layout*	always needs to be AMICI_BLAS_ColMajor.
in	*TransA*	flag indicating whether A should be transposed before multiplication
in	*M*	number of rows in A
in	*N*	number of columns in A
in	*alpha*	coefficient alpha
in	*A*	matrix A
in	*lda*	leading dimension of A (m or n)
in	*X*	vector X
in	*incX*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

Returns

void

Definition at line 398 of file amici_interface_matlab.cpp.

Here is the call graph for this function:



10.6.3.6 expDataFromMatlabCall()

```
ExpData* expDataFromMatlabCall (
            const mxArray * prhs[ ],
            const UserData * udata,
            Model * model )
```

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

Parameters

in	*prhs*	pointer to the array of input arguments **Type**: mxArray
in	*udata*	pointer to user data object **Type**: UserData
in	*model*	pointer to the model object, this is necessary to perform dimension checks **Type**: Model

Returns

edata pointer to experimental data object
Type: ExpData

Definition at line 426 of file amici_interface_matlab.cpp.

10.7 src/spline.cpp File Reference

definition of spline functions

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

10.7.1 Detailed Description

Author

Peter & Nigel, Design Software, 42 Gubberley St, Kenmore, 4069, Australia.

10.7.2 Function Documentation

10.7.2.1 spline()

```
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

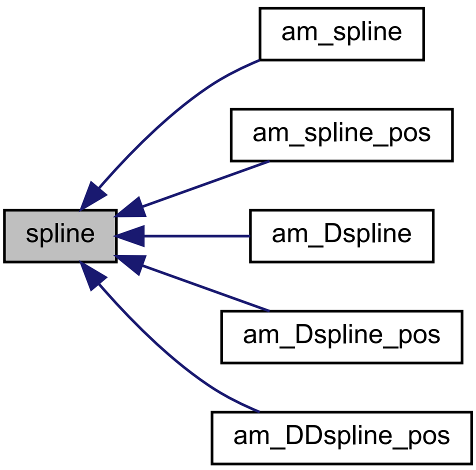
0	normal return
1	less than two data points; cannot interpolate
2	x[] are not in ascending order

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 65 of file spline.cpp.

Here is the caller graph for this function:



10.7.2.2 seval()

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

Evaluate 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] 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

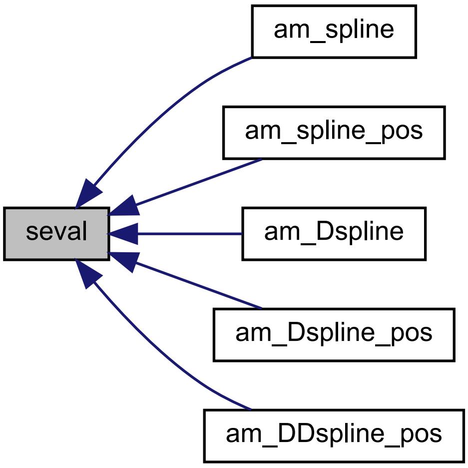
the value of the spline function at u

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 197 of file spline.cpp.

Here is the caller graph for this function:



10.7.2.3 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.

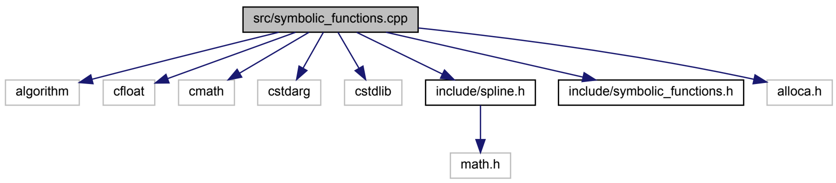
Definition at line 258 of file spline.cpp.

10.8 src/symbolic_functions.cpp File Reference

definition of symbolic functions

```
#include <algorithm>
#include <cfloat>
#include <cmath>
#include <cstdarg>
#include <cstdlib>
#include <include/spline.h>
#include <include/symbolic_functions.h>
#include <alloca.h>
```

Include dependency graph for symbolic_functions.cpp:



Functions

- int amiIsNaN (double what)
- int amiIsInf (double what)
- double amiGetNaN ()
- double amilog (double x)
- double dirac (double x)
- double heaviside (double x)
- double sign (double x)
- double am_min (double a, double b, double c)
- double Dam_min (int id, double a, double b, double c)
- double am_max (double a, double b, double c)
- double Dam_max (int id, double a, double b, double c)
- double am_spline (double t, int num,...)
- double am_spline_pos (double t, int num,...)
- double am_Dspline (int id, double t, int num,...)
- double am_Dspline_pos (int id, double t, int num,...)
- double am_DDspline (int id1, int id2, double t, int num,...)
- double am_DDspline_pos (int id1, int id2, double t, int num,...)

10.8.1 Detailed Description

This file contains definitions of various symbolic functions which

10.8.2 Function Documentation

10.8.2.1 amiIsNaN()

```
int amiIsNaN (
            double what )
```

c++ interface to the isNaN function

Parameters

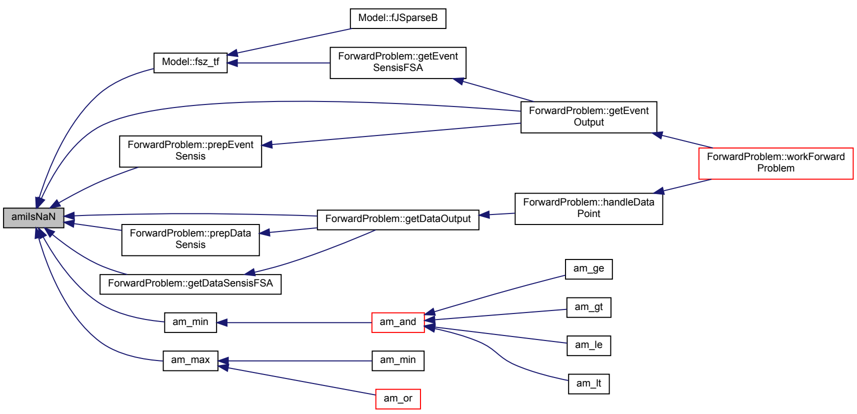
what	argument

Returns

isnan(what)

Definition at line 32 of file symbolic_functions.cpp.

Here is the caller graph for this function:



10.8.2.2 amiIsInf()

```
int amiIsInf (
            double what )
```

c++ interface to the isinf function

Parameters

what	argument

Returns

isnan(what)

Definition at line 43 of file symbolic_functions.cpp.

10.8.2.3 amiGetNaN()

```
double amiGetNaN ( )
```

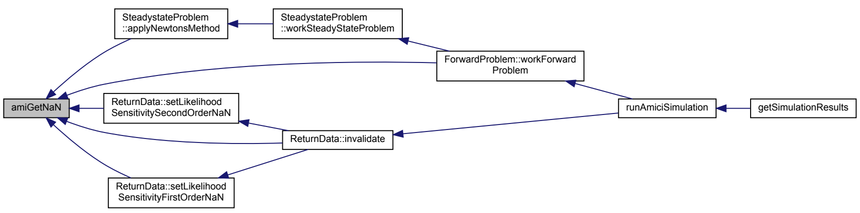
function returning nan

Returns

NaN

Definition at line 53 of file symbolic_functions.cpp.

Here is the caller graph for this function:



10.8.2.4 amilog()

```
double amilog (
            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 65 of file symbolic_functions.cpp.

10.8.2.5 dirac()

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

c implementation of matlab function dirac

Parameters

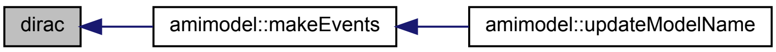
x	argument

Returns

if(x==0) then INF else 0

Definition at line 80 of file symbolic_functions.cpp.

Here is the caller graph for this function:



10.8.2.6 heaviside()

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

c implementation of matlab function heaviside

Parameters

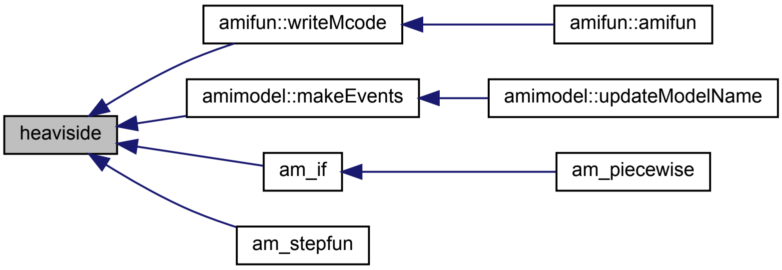
x	argument

Returns

if(x>0) then 1 else 0

Definition at line 95 of file symbolic_functions.cpp.

Here is the caller graph for this function:



10.8.2.7 sign()

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

c implementation of matlab function sign

Parameters

x	argument

Returns

0
Type: double

Definition at line 110 of file symbolic_functions.cpp.

10.8.2.8 am_min()

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

c implementation of matlab function min

Parameters

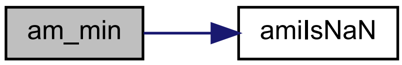
a	value1 **Type**: double
b	value2 **Type**: double
c	bogus parameter to ensure correct parsing as a function **Type**: double

Returns

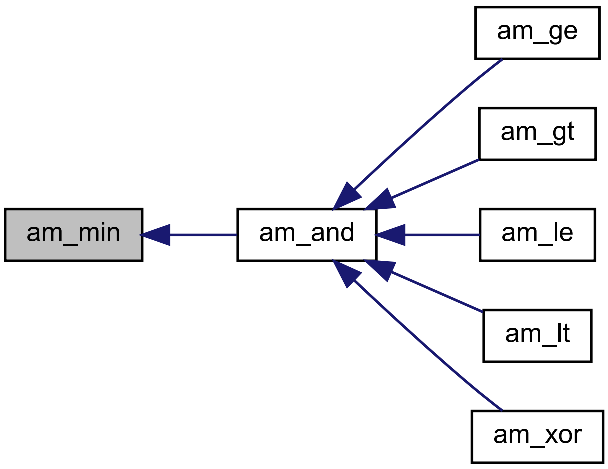
if(a < b) then a else b
Type: double

Definition at line 131 of file symbolic_functions.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.8.2.9 Dam_min()

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

parameter derivative of c implementation of matlab function min

Parameters

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

Returns

id == 1: if(a $<$ b) then 1 else 0
Type: double
id == 2: if(a $<$ b) then 0 else 1
Type: double

Definition at line 154 of file symbolic_functions.cpp.

10.8.2.10 am_max()

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

c implementation of matlab function max

Parameters

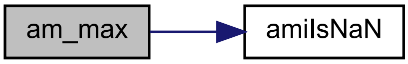
a	value1 **Type**: double
b	value2 **Type**: double
c	bogus parameter to ensure correct parsing as a function **Type**: double

Returns

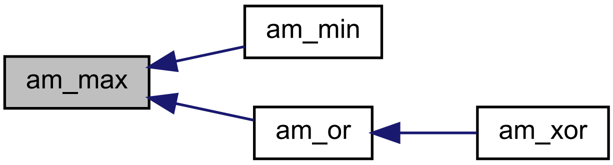
if(a $>$ b) then a else b
Type: double

Definition at line 179 of file symbolic_functions.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



10.8.2.11 Dam_max()

```
double Dam_max (
            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 **Type**: double
b	value2 **Type**: double
c	bogus parameter to ensure correct parsing as a function **Type**: double

Returns

id == 1: if(a $>$ b) then 1 else 0
Type: double

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

Definition at line 202 of file symbolic_functions.cpp.

10.8.2.12 am_spline()

```
double am_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

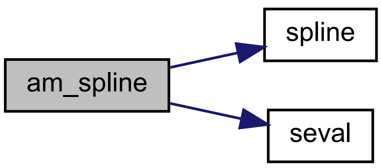
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

spline(t)

Definition at line 229 of file symbolic_functions.cpp.

Here is the call graph for this function:



10.8.2.13 am_spline_pos()

```
double am_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

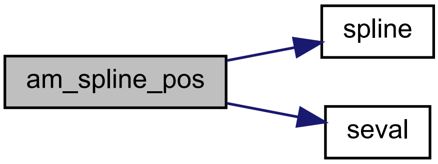
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

spline(t)

Definition at line 280 of file symbolic_functions.cpp.

Here is the call graph for this function:



10.8.2.14 am_Dspline()

```
double am_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

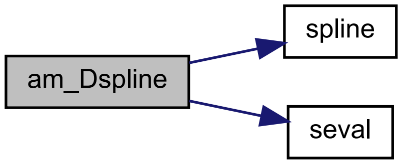
id	index of node to which the derivative of the corresponding spline coefficient should be computed
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

dsplinedp(t)

Definition at line 332 of file symbolic_functions.cpp.

Here is the call graph for this function:



10.8.2.15 am_Dspline_pos()

```
double am_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

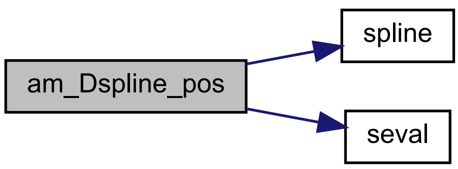
id	index of node to which the derivative of the corresponding spline coefficient should be computed
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

dsplinedp(t)

Definition at line 388 of file symbolic_functions.cpp.

Here is the call graph for this function:



10.8.2.16 am_DDspline()

```
double am_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 453 of file symbolic_functions.cpp.

10.8.2.17 am_DDspline_pos()

```
double am_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

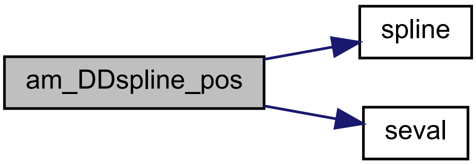
id1	index of node to which the first derivative of the corresponding spline coefficient should be computed
id2	index of node to which the second derivative of the corresponding spline coefficient should be computed
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

ddspline(t)

Definition at line 468 of file symbolic_functions.cpp.

Here is the call graph for this function:



10.9 symbolic/am_and.m File Reference

am_and is the amici implementation of the symbolic and function

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_and (::sym a,::sym b)

    am_and is the amici implementation of the symbolic and function

10.9.1 Function Documentation

10.9.1.1 am_and()

```
mlhsInnerSubst< matlabtypesubstitute > am_and (
            ::sym a,
            ::sym b )
```

Parameters

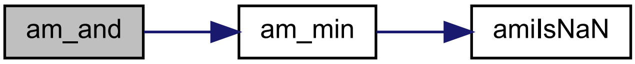
a	first input parameter
b	second input parameter

Return values

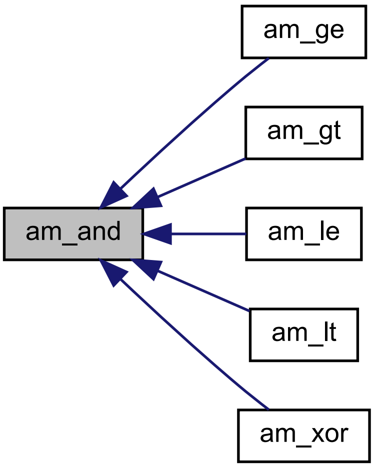
fun	logical value, negative for false, positive for true

Definition at line 17 of file am_and.m.

Here is the call graph for this function:



Here is the caller graph for this function:



10.10 symbolic/am_eq.m File Reference

am_eq is currently a placeholder that simply produces an error message

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_eq (matlabtypesubstitute varargin)
  am_eq is currently a placeholder that simply produces an error message

10.10.1 Function Documentation

10.10.1.1 am_eq()

```
mlhsInnerSubst< matlabtypesubstitute > am_eq (
            matlabtypesubstitute varargin )
```

Parameters

varargin	elements for chain of equalities

Return values

fun	logical value, negative for false, positive for true

Definition at line 17 of file am_eq.m.

10.11 symbolic/am_ge.m File Reference

am_ge is the amici implementation of the n-ary mathml greaterorequal function this is an n-ary function, for more than 2 input parameters it will check whether and(varargin{1} >= varargin{2},varargin{2} >= varargin{3},...)

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_ge (::sym varargin)

    am_ge is the amici implementation of the n-ary mathml greaterorequal function this is an n-ary function, for more than 2 input parameters it will check whether and(varargin{1} >= varargin{2},varargin{2} >= varargin{3},...)

10.11.1 Function Documentation

10.11.1.1 am_ge()

```
mlhsInnerSubst< matlabtypesubstitute > am_ge (
            ::sym varargin )
```

Parameters

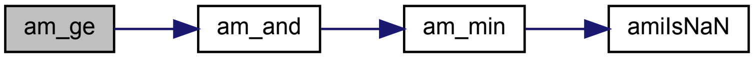
varargin	chain of input parameters

Return values

fun	a >= b logical value, negative for false, positive for true

Definition at line 17 of file am_ge.m.

Here is the call graph for this function:



10.12 symbolic/am_gt.m File Reference

am_gt is the amici implementation of the n-ary mathml greaterthan function this is an n-ary function, for more than 2 input parameters it will check whether and(varargin{1} > varargin{2},varargin{2} > varargin{3},...)

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_gt (::sym varargin)

    am_gt is the amici implementation of the n-ary mathml greaterthan function this is an n-ary function, for more than 2 input parameters it will check whether and(varargin{1} > varargin{2},varargin{2} > varargin{3},...)

10.12.1 Function Documentation

10.12.1.1 am_gt()

```
mlhsInnerSubst< matlabtypesubstitute > am_gt (
            ::sym varargin )
```

Parameters

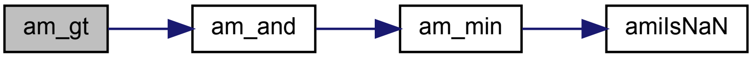
varargin	chain of input parameters

Return values

fun	a > b logical value, negative for false, positive for true

Definition at line 17 of file am_gt.m.

Here is the call graph for this function:



10.13 symbolic/am_if.m File Reference

am_if is the amici implementation of the symbolic if function

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_if (::sym condition,::sym truepart,::sym falsepart)
  am_if is the amici implementation of the symbolic if function

10.13.1 Function Documentation

10.13.1.1 am_if()

```
mlhsInnerSubst< matlabtypesubstitute > am_if (
            ::sym condition,
            ::sym truepart,
            ::sym falsepart )
```

Parameters

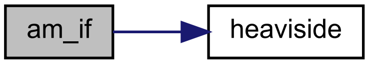
condition	logical value
truepart	value if condition is true
falsepart	value if condition is false

Return values

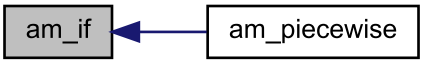
fun	if condition is true truepart, else falsepart

Definition at line 17 of file am_if.m.

Here is the call graph for this function:



Here is the caller graph for this function:



10.14 symbolic/am_le.m File Reference

am_le is the amici implementation of the n-ary mathml lessorequal function this is an n-ary function, for more than 2 input parameters it will check whether and(varargin{1} <= varargin{2},varargin{2} <= varargin{3},...)

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_le (::sym varargin)

  am_le is the amici implementation of the n-ary mathml lessorequal function this is an n-ary function, for more than 2 input parameters it will check whether and(varargin{1} <= varargin{2},varargin{2} <= varargin{3},...)

10.14.1 Function Documentation

10.14.1.1 am_le()

```
mlhsInnerSubst< matlabtypesubstitute > am_le (
            ::sym varargin )
```

Parameters

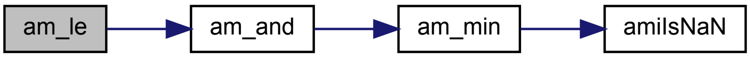
varargin	chain of input parameters

Return values

fun	a <= b logical value, negative for false, positive for true

Definition at line 17 of file am_le.m.

Here is the call graph for this function:



10.15 symbolic/am_lt.m File Reference

am_lt is the amici implementation of the n-ary mathml lessthan function this is an n-ary function, for more than 2 input parameters it will check whether and(varargin{1} < varargin{2},varargin{2} < varargin{3},...)

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_lt (::sym varargin)

  am_lt is the amici implementation of the n-ary mathml lessthan function this is an n-ary function, for more than 2 input parameters it will check whether and(varargin{1} < varargin{2},varargin{2} < varargin{3},...)

10.15.1 Function Documentation

10.15.1.1 am_lt()

```
mlhsInnerSubst< matlabtypesubstitute > am_lt (
            ::sym varargin )
```

Parameters

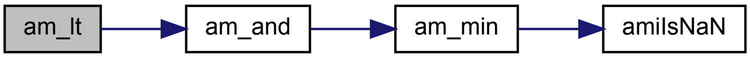
varargin	chain of input parameters

Return values

fun	a < b logical value, negative for false, positive for true

Definition at line 17 of file am_lt.m.

Here is the call graph for this function:



10.16 symbolic/am_max.m File Reference

am_max is the amici implementation of the symbolic max function

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_max (::sym a,::sym b)
  am_max is the amici implementation of the symbolic max function

10.16.1 Function Documentation

10.16.1.1 am_max()

```
mlhsInnerSubst< matlabtypesubstitute > am_max (
             ::sym a,
             ::sym b )
```

Parameters

a	first input parameter
b	second input parameter

Return values

fun	maximum of a and b

Definition at line 17 of file am_max.m.

10.17 symbolic/am_min.m File Reference

am_min is the amici implementation of the symbolic min function

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_min (::sym a,::sym b)
  am_min is the amici implementation of the symbolic min function

10.17.1 Function Documentation

10.17.1.1 am_min()

```
mlhsInnerSubst< matlabtypesubstitute > am_min (
            ::sym a,
            ::sym b )
```

Parameters

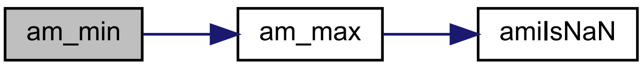
a	first input parameter
b	second input parameter

Return values

fun	minimum of a and b

Definition at line 17 of file am_min.m.

Here is the call graph for this function:



10.18 symbolic/am_or.m File Reference

am_or is the amici implementation of the symbolic or function

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_or (::sym a,::sym b)
  am_or is the amici implementation of the symbolic or function

10.18.1 Function Documentation

10.18.1.1 am_or()

```
mlhsInnerSubst< matlabtypesubstitute > am_or (
            ::sym a,
            ::sym b )
```

Parameters

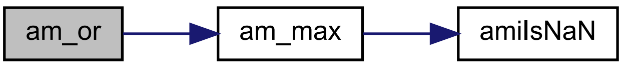
a	first input parameter
b	second input parameter

Return values

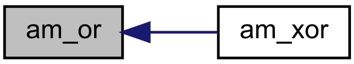
fun	logical value, negative for false, positive for true

Definition at line 17 of file am_or.m.

Here is the call graph for this function:



Here is the caller graph for this function:



10.19 symbolic/am_piecewise.m File Reference

am_piecewise is the amici implementation of the mathml piecewise function

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_piecewise (matlabtypesubstitute piece, matlabtypesubstitute condition, matlabtypesubstitute default)

    am_piecewise is the amici implementation of the mathml piecewise function

10.19.1 Function Documentation

10.19.1.1 am_piecewise()

```
mlhsInnerSubst< matlabtypesubstitute > am_piecewise (
            matlabtypesubstitute piece,
            matlabtypesubstitute condition,
            matlabtypesubstitute default )
```

Parameters

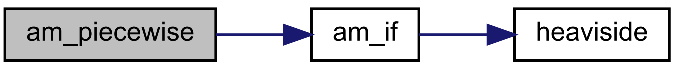
piece	value if condition is true
condition	logical value
default	value if condition is false

Return values

fun	return value, piece if condition is true, default if not

Definition at line 17 of file am_piecewise.m.

Here is the call graph for this function:



10.20 symbolic/am_stepfun.m File Reference

am_stepfun is the amici implementation of the step function

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_stepfun (::sym t, matlabtypesubstitute tstart, matlabtypesubstitute vstart, matlabtypesubstitute tend, matlabtypesubstitute vend)

    am_stepfun is the amici implementation of the step function

10.20.1 Function Documentation

10.20.1.1 am_stepfun()

```
mlhsInnerSubst< matlabtypesubstitute > am_stepfun (
            ::sym t,
            matlabtypesubstitute tstart,
            matlabtypesubstitute vstart,
            matlabtypesubstitute tend,
            matlabtypesubstitute vend )
```

Parameters

t	input variable
tstart	input variable value at which the step starts
vstart	value during the step
tend	input variable value at which the step end
vend	value after the step

Return values

fun	0 before tstart, vstart between tstart and tend and vend after tend

Definition at line 17 of file am_stepfun.m.

Here is the call graph for this function:

10.21 symbolic/am_xor.m File Reference

am_xor is the amici implementation of the symbolic exclusive or function

Functions

- mlhsInnerSubst< matlabtypesubstitute > am_xor (::sym a,::sym b)

  am_xor is the amici implementation of the symbolic exclusive or function

10.21.1 Function Documentation

10.21.1.1 am_xor()

```
mlhsInnerSubst< matlabtypesubstitute > am_xor (
            ::sym a,
            ::sym b )
```

Parameters

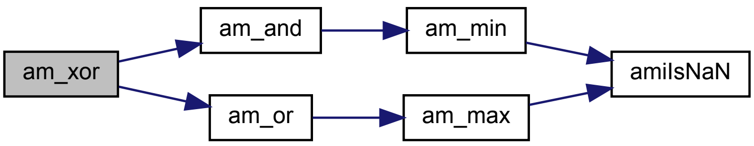
a	first input parameter
b	second input parameter

Return values

fun	logical value, negative for false, positive for true

Definition at line 17 of file am_xor.m.

Here is the call graph for this function:



10.22 tests/cpputest/createTestingData.m File Reference

createTestingData runs simulation on all test models and writes results as hdf5. currently necessary for continuous integration to yield meaningful results

Functions

- noret::substitute createTestingData ()
  createTestingData runs simulation on all test models and writes results as hdf5. currently necessary for continuous integration to yield meaningful results

10.23 tests/cpputest/wrapTestModels.m File Reference

wrapTestModels calls amiwrap on all test models. currently necessary for continuous integrations to yield meaningful results

Functions

- noret::substitute wrapTestModels ()

  wrapTestModels calls amiwrap on all test models. currently necessary for continuous integrations to yield meaningful results

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