AMICI

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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

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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, lain 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

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 Model Definition 5

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 unknown 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 function 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 Model Simulation 9

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/*.cpp, 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:

amievent	77
amifun	??
BackwardProblem	??
ExpData	??
ForwardProblem handle	??
amidata	??
amimodel	??
amised	??
SBMLode CustomDisplay	??
amioption	??
Model	??
modelTest	??
NewtonSolver	??
NewtonSolverDense	??
NewtonSolverIterative	??
NewtonSolverSparse	??

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	ReturnData	??
	ReturnDataMatlab	??
	SteadystateProblem sym	??
	optsym	??
	TempData	??
	UserData	??
8	Class Index	
8.	1 Class List	
Н	ere are the classes, structs, unions and interfaces with brief descriptions:	
	amidata 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	??
	amievent AMIEVENT defines events which later on will be transformed into appropriate C code	??
	amifun AMIFUN defines functions which later on will be transformed into appropriate C code	??
	amimodel AMIMODEL carries all model definitions including functions and events	??
	amioption AMIOPTION provides an option container to pass simulation parameters to the simulation routine	?1
	amised AMISED is a container for SED-ML objects	??
	BackwardProblem Class to solve backwards problems	??
	ExpData Struct that carries all information about experimental data	??
	ForwardProblem Groups all functions for solving the backwards problem. Has only static members	??
	Model AMICI ODE model. The model does not contain any data, its state should never change	??
	modelTest MODELTEST Summary of this class goes here Detailed explanation goes here	??
	NewtonSolver	??
	NewtonSolverDense	??

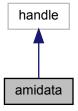
NewtonSolverIterative	??
NewtonSolverSparse	??
optsym OPTSYM is an auxiliary class to gain access to the private symbolic property s which is necessary to be able to call symobj::optimize on it	??
ReturnData Struct that stores all data which is later returned by the mex function	??
ReturnDataMatlab Sets up ReturnData to be returned by the MATLAB mex functions. Memory is allocated using matlab functions	??
SBMLode SBMLMODEL provides an intermediate container between the SBML definition and an amimodel object	??
SteadystateProblem Solves a steady-state problem using Newton's method and falls back to integration on failure	??
TempData Struct that provides temporary storage for different variables	??
UserData Struct that stores all user provided data	??

9 Class Documentation

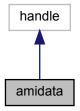
9.1 amidata Class Reference

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()  \label{eq:amidata} \mbox{amidata (} \\  \mbox{matlabtypesubstitute } \mbox{\it 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("")
```

Definition at line 95 of file amidata.m.

This property has custom functionality when its value is changed.

Note

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 (  \mbox{ matlabtypesubstitute } trigger, \\ \mbox{ matlabtypesubstitute } bolus, \\ \mbox{ matlabtypesubstitute } z \mbox{ )}
```

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	
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()

Parameters

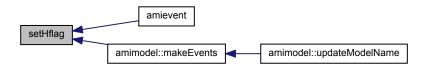
hflag	value for the hflag property
-------	------------------------------

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

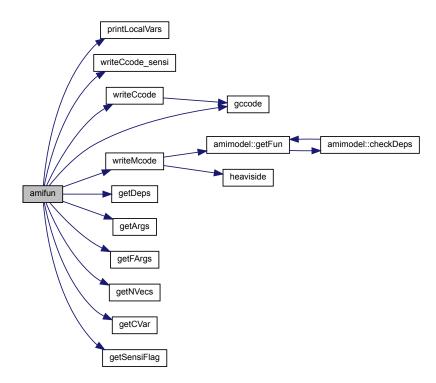
```
9.3.2.1 amifun()
```

Parameters

funstr name of the requested function		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

mode	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:



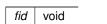
9.3.3.2 writeCcode_sensi()

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

Parameters

	model	model model defintion object	
fid file id in which the final expression is wr		file id in which the final expression is written	1

Return values



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		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

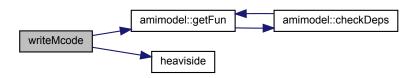
model model defintion object

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

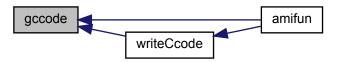
model	model definition object
fid	file id in which the expression should be written

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("")
```

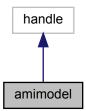
Default: logical.empty("")

Definition at line 107 of file amifun.m.

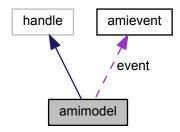
9.4 amimodel Class Reference

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 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 sensitiv-
     ities (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 expres-
```

sions

• ::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()

Parameters

symfun	this is the string to the function which generates the modelstruct. You can also directly pass the struct here	the
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()

```
\label{eq:noret::substitute updateRHS (} $$ matlabtypesubstitute $xdot $ ) $
```

Parameters

xdot new right hand side of the differential equation

Definition at line 623 of file amimodel.m.

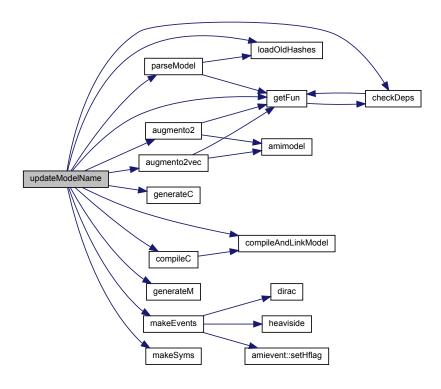
9.4.3.2 updateModelName()

Parameters

modelname new modelr

Definition at line 636 of file amimodel.m.

Here is the call graph for this function:



9.4.3.3 generateC()

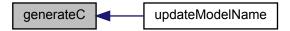
```
noret::substitute generateC ( )
```

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()

Parameters

amimodelo2

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

Return values

this model definition object	t
------------------------------	---

Definition at line 18 of file generateM.m.

Here is the caller graph for this function:



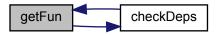
9.4.3.6 getFun()

Parameters

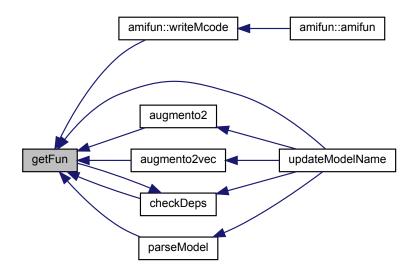
HTable	struct with hashes of symbolic definition from the previous compilation
funstr	function for which symbolic expressions should be computed

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()

Parameters

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

Return values

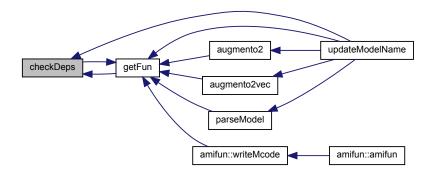
cflag	boolean indicating whether any of the dependencies have changed with respect to the hashes stored in
	HTable

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()

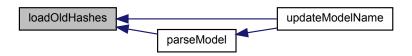
mlhsInnerSubst<::struct > loadOldHashes ()

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()

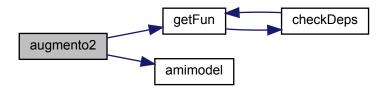
 $\verb|mlhsInnerSubst| < \verb|matlabtypesubstitute| > \verb|augmento2| ()$

Return values

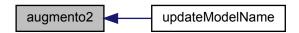
this | augmented system which contains symbolic definition of the original system and its sensitivities

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()

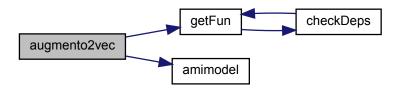
```
mlhsInnerSubst< matlabtypesubstitute > augmento2vec ( )
```

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()

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 =
    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 =
    Matlab documentation of property attributes.
```

Definition at line 83 of file amimodel.m.

Default: false

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 =
    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 =
    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 =

Definition at line 215 of file amimodel.m.

Default: double.empty("")

Matlab documentation of property attributes.

Public

```
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 =
    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 =
    Matlab documentation of property attributes.
    Default: double.empty("")
Definition at line 292 of file amimodel.m.
9.4.4.26 sparseidx
sparseidx = double.empty("")
```

```
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 =
    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 =

Definition at line 347 of file amimodel.m.

Default: double.empty("")

Matlab documentation of property attributes.

```
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 = "-03"
```

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 =
    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 =
    Matlab documentation of property attributes.
```

Definition at line 435 of file amimodel.m.

Default: struct.empty("")

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

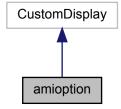
Default: 0

Definition at line 515 of file amimodel.m.

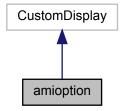
9.5 amioption Class Reference

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 Imm = 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 ImmB = 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 = 0Default: 0 Definition at line 76 of file amioption.m. 9.5.3.8 lmm lmm = 2Default: 2 Definition at line 84 of file amioption.m. 9.5.3.9 iter iter = 2Default: 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 ImmB lmmB = 2Default: 2 Definition at line 124 of file amioption.m. 9.5.3.14 iterB

Default: 2

iterB = 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.

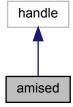
Default: double.empty("")

Definition at line 260 of file amioption.m.

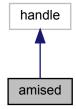
9.6 amised Class Reference

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

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 =
    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 =
    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()

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

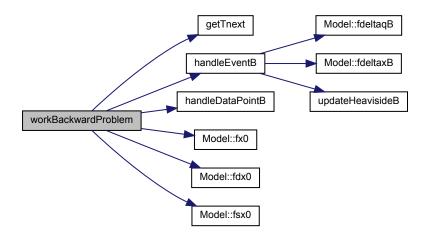
in	udata	pointer to the user data struct Type : UserData
in	tdata	pointer to the temporary data struct Type : TempData
out	rdata	pointer to the return data struct Type : ReturnData
in	model	pointer to model specification object Type: Model

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

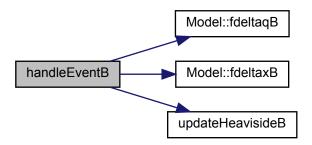
Returns

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()

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.



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()

initialization with UserData and model

Definition at line 9 of file edata.cpp.



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

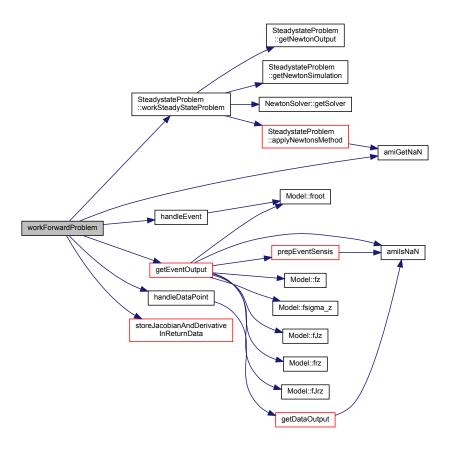
Returns

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

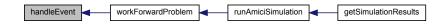
Type: int

Definition at line 123 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



$9.9.2.3 \quad store Jacobian And Derivative In Return Data () \\$

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

Parameters

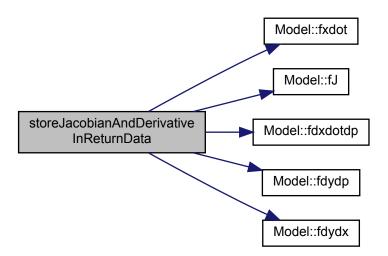
out	tdata	pointer to the temporary data struct Type : TempData
out	rdata	pointer to the return data struct Type : ReturnData
in	model	pointer to model specification object Type: Model

Returns

void

Definition at line 321 of file forwardproblem.cpp.

Here is the call graph for this function:





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

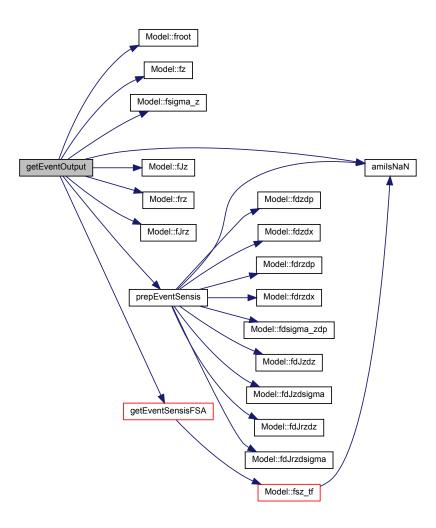
Returns

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

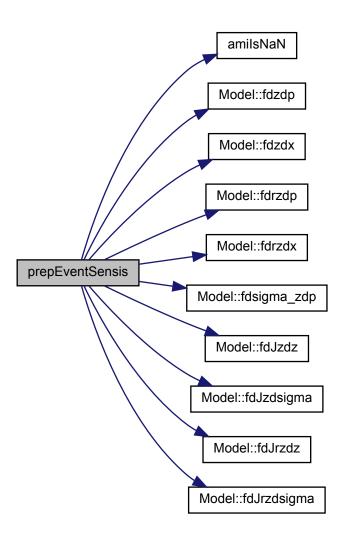
Returns

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()

```
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

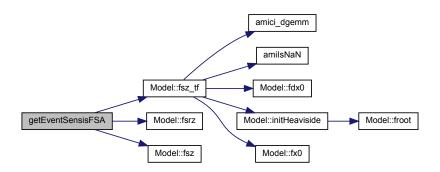
Returns

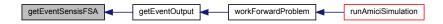
status flag indicating success of execution

Type: int

Definition at line 608 of file forwardproblem.cpp.

Here is the call graph for this function:





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

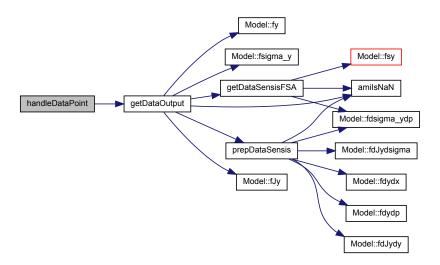
Returns

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

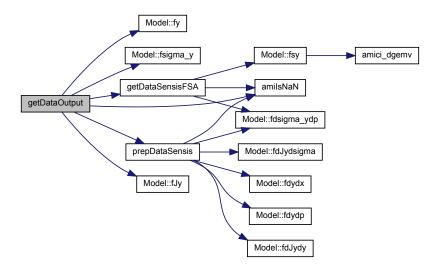
Returns

status flag indicating success of execution

Type: int

Definition at line 690 of file forwardproblem.cpp.

Here is the call graph for this function:





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

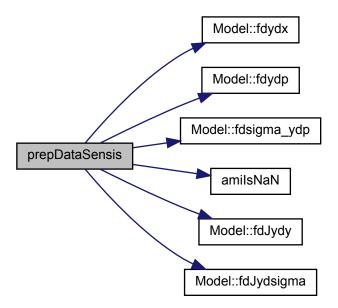
Returns

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

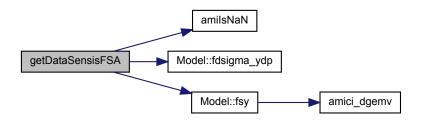
out	status	flag indicating success of execution Type : int
in	it	index of current timepoint Type: int
in	udata	pointer to the user data struct Type : UserData
out	rdata	pointer to the return data struct Type : ReturnData
in	edata	pointer to the experimental data struct Type : ExpData
out	tdata	pointer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

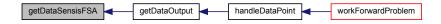
Returns

void

Definition at line 833 of file forwardproblem.cpp.

Here is the call graph for this function:





9.9.2.11 applyEventBolus()

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()

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()

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 ()=0
- 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,
- 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, SIsMat 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, SIsMat 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

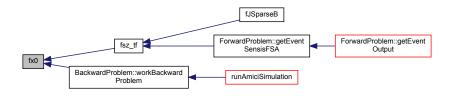
9.10.2.1 fx0()

```
virtual int fx0 ( N_{void} * user_{data} ) [virtual]
```

Initial states

Definition at line 33 of file amici_model.h.

Here is the caller graph for this function:



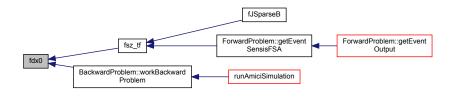
9.10.2.2 fdx0()

```
virtual int fdx0 (  \begin{tabular}{ll} N\_Vector $x0$, \\ N\_Vector $dx0$, \\ void * user\_data ) & [virtual] \end{tabular}
```

Initial value for time derivative of states

Definition at line 36 of file amici_model.h.

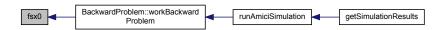
Here is the caller graph for this function:



9.10.2.3 fsx0()

Initial value for time derivative of states

Definition at line 41 of file amici_model.h.



9.10.2.4 fsdx0()

```
virtual int fsdx0 (  & \text{N\_Vector} * sdx0, \\ & \text{N\_Vector} x, \\ & \text{N\_Vector} dx, \\ & \text{void} * user\_data ) \quad \text{[virtual]}
```

Sensitivity of initial states x0

Definition at line 44 of file amici_model.h.

9.10.2.5 fJ()

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()

Jacobian of xBdot with respect to adjoint state xB

Definition at line 50 of file amici_model.h.

9.10.2.7 fJDiag()

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()

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

Definition at line 56 of file amici_model.h.



9.10.2.9 froot()

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.



9.10.2.11 fsrz()

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()

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.



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:

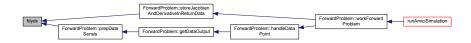


9.10.2.15 fdydx()

```
virtual int fdydx (  real type \ 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.



9.10.2.16 fz()

Event-resolved measurements

Definition at line 80 of file amici_model.h.

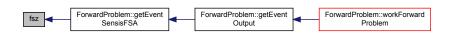
Here is the caller graph for this function:



9.10.2.17 fsz()

Sensitivity of z, total derivative

Definition at line 83 of file amici_model.h.



9.10.2.18 fdzdp()

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()

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

Definition at line 89 of file amici_model.h.



9.10.2.20 fdrzdp()

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()

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

Definition at line 95 of file amici_model.h.

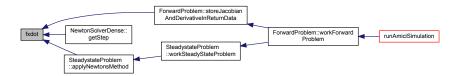


9.10.2.22 fxdot()

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()

Right hand side of differential equation for adjoint state xB

Definition at line 101 of file amici model.h.

9.10.2.24 fqBdot()

Right hand side of integral equation for quadrature states qB

Definition at line 104 of file amici_model.h.

9.10.2.25 fdxdotdp()

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()

State update functions for events

Definition at line 110 of file amici_model.h.



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()

Adjoint state update functions for events

Definition at line 116 of file amici_model.h.



9.10.2.29 fdeltaqB()

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 (  \mbox{realtype } t, \\ \mbox{TempData } * tdata \; ) \quad \mbox{[virtual]}
```

Standard deviation of measurements

Definition at line 122 of file amici_model.h.

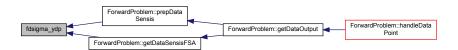


9.10.2.31 fdsigma_ydp()

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()

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.



9.10.2.34 fJy()

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()

negative log-likelihood of event-resolved measurements \boldsymbol{z}

Definition at line 137 of file amici_model.h.



9.10.2.36 fJrz()

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:

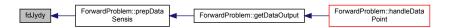


9.10.2.37 fdJydy()

```
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.



9.10.2.38 fdJydsigma()

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()

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

Definition at line 149 of file amici_model.h.



9.10.2.40 fdJzdsigma()

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()

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.



9.10.2.42 fdJrzdsigma()

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()

Right hand side of differential equation for state sensitivities sx

Definition at line 161 of file amici_model.h.

9.10.2.44 fJSparse()

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()

J in banded form (for banded solvers)

Definition at line 167 of file amici_model.h.

9.10.2.46 fJBandB()

JB in banded form (for banded solvers)

Definition at line 170 of file amici_model.h.

9.10.2.47 fJvB()

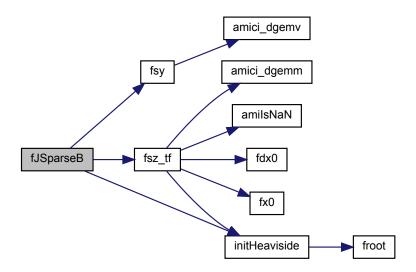
Matrix vector product of JB with a vector v (for iterative solvers)

Definition at line 173 of file amici_model.h.

9.10.2.48 fJSparseB()

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

Definition at line 176 of file amici_model.h.



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:

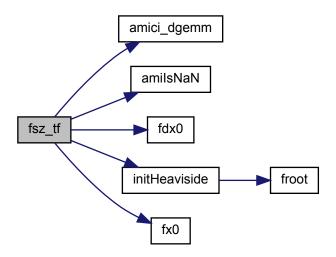


```
9.10.2.50 fsz_tf()
```

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()

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

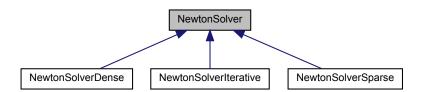
MODELTEST Summary of this class goes here Detailed explanation goes here.

9.11.1 Detailed Description

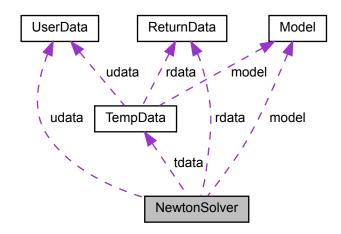
Definition at line 17 of file modelTest.m.

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, Temp-Data *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()

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()

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

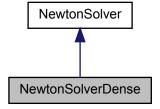
Implemented in NewtonSolverIterative, NewtonSolverSparse, and NewtonSolverDense.

Here is the caller graph for this function:

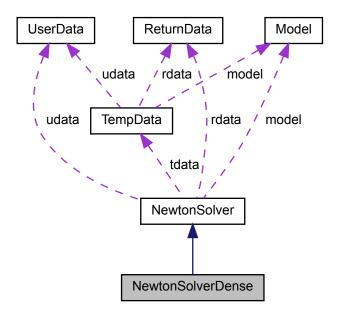


9.13 NewtonSolverDense Class Reference

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()

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

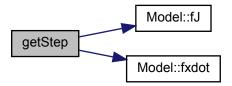
int status flag indicating success of execution

Type: int

Implements NewtonSolver.

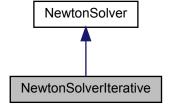
Definition at line 95 of file newton_solver.cpp.

Here is the call graph for this function:

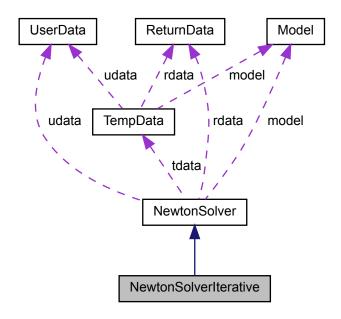


9.14 NewtonSolverIterative Class Reference

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()

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.

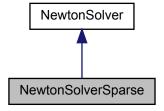
Definition at line 189 of file newton_solver.cpp.

Here is the call graph for this function:

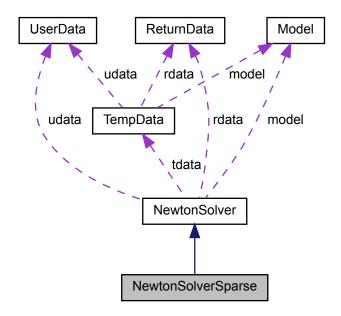


9.15 NewtonSolverSparse Class Reference

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()

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.

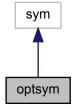
Here is the call graph for this function:



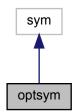
9.16 optsym Class Reference

OPTSYM is an auxiliary class to gain access to the private symbolic property ${\tt s}$ 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()

```
{\tt mlhsInnerSubst}{<}{\tt ::}{\tt sym} \,>\, {\tt getoptimized} \ (\ )
```

Return values

out optimized symbolic object

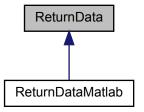
Definition at line 42 of file optsym.m.

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 (const UserData *udata, const Model *model)
- virtual void setDefaults ()
- void invalidate ()

performs all necessary actions to reset return data upon integration failure

- void setLikelihoodSensitivityFirstOrderNaN ()
- void setLikelihoodSensitivitySecondOrderNaN ()
- int applyChainRuleFactorToSimulationResults (const UserData *udata, const realtype *unscaledParameters)

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 * IIh
- 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 Member Function Documentation

9.17.2.1 invalidate()

void invalidate ()

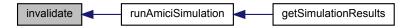
Parameters

in	udata	pointer to the user data struct
		Type: UserData

Definition at line 45 of file rdata.cpp.

Here is the call graph for this function:





9.17.2.2 initField2()

@ brief initialise matrix and attach to the field @ param FIELD name of the field to which the matrix will be attached @ param D1 number of rows in the matrix @ param D2 number of columns in the matrix

Reimplemented in ReturnDataMatlab.

Definition at line 408 of file rdata.cpp.

9.17.2.3 initField3()

@ brief initialise 3D tensor and attach to the field @ param FIELD name of the field to which the tensor will be attached @ param D1 number of rows in the tensor @ param D2 number of columns in the tensor @ param D3 number of elements in the third dimension of the tensor

Reimplemented in ReturnDataMatlab.

Definition at line 413 of file rdata.cpp.

9.17.2.4 initField4()

@ brief initialise 4D tensor and attach to the field @ param FIELD name of the field to which the tensor will be attached @ param D1 number of rows in the tensor @ param D2 number of columns in the tensor @ param D3 number of elements in the third dimension of the tensor @ param D4 number of elements in the fourth dimension of the tensor

Reimplemented in ReturnDataMatlab.

Definition at line 418 of file rdata.cpp.

9.17.3 Member Data Documentation 9.17.3.1 ts double* ts timepoints (dimension: nt) Definition at line 38 of file rdata.h. 9.17.3.2 xdot double* xdot time derivative (dimension: nx) Definition at line 41 of file rdata.h. 9.17.3.3 dxdotdp double* dxdotdp parameter derivative of time derivative (dimension: nx x nplist, column-major) Definition at line 45 of file rdata.h. 9.17.3.4 dydx double* dydx state derivative of observables (dimension: ny x nx, column-major) Definition at line 48 of file rdata.h.

9.17.3.5 dydp

double* dydp

Definition at line 52 of file rdata.h.

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

```
9.17.3.6 J
double* J
Jacobian of differential equation right hand side (dimension: nx x nx, column-major)
Definition at line 56 of file rdata.h.
9.17.3.7 z
double* z
event output (dimension: nmaxevent x nz, column-major)
Definition at line 59 of file rdata.h.
9.17.3.8 sigmaz
double* sigmaz
event output sigma standard deviation (dimension: nmaxevent x nz, column-major)
Definition at line 63 of file rdata.h.
9.17.3.9 sz
double* sz
parameter derivative of event output (dimension: nmaxevent x nz, column-major)
Definition at line 67 of file rdata.h.
9.17.3.10 ssigmaz
double* ssigmaz
parameter derivative of event output standard deviation (dimension: nmaxevent x nz, column-major)
Definition at line 71 of file rdata.h.
```

```
9.17.3.11 rz
double* rz
event trigger output (dimension: nmaxevent x nz, column-major)
Definition at line 74 of file rdata.h.
9.17.3.12 srz
double* srz
parameter derivative of event trigger output (dimension: nmaxevent x nz x nplist, column-major)
Definition at line 78 of file rdata.h.
9.17.3.13 s2rz
double* s2rz
second order parameter derivative of event trigger output (dimension: nmaxevent x nztrue x nplist x nplist, column-
major)
Definition at line 82 of file rdata.h.
9.17.3.14 x
double* x
state (dimension: nt x nx, column-major)
Definition at line 85 of file rdata.h.
9.17.3.15 sx
double* sx
parameter derivative of state (dimension: nt x nx x nplist, column-major)
Definition at line 89 of file rdata.h.
```

```
9.17.3.16 y
double* y
observable (dimension: nt x ny, column-major)
Definition at line 92 of file rdata.h.
9.17.3.17 sigmay
double* sigmay
observable standard deviation (dimension: nt x ny, column-major)
Definition at line 95 of file rdata.h.
9.17.3.18 sy
double* sy
parameter derivative of observable (dimension: nt x ny x nplist, column-major)
Definition at line 99 of file rdata.h.
9.17.3.19 ssigmay
double* ssigmay
parameter derivative of observable standard deviation (dimension: nt x ny x nplist, column-major)
Definition at line 103 of file rdata.h.
9.17.3.20 numsteps
double* numsteps
number of integration steps forward problem (dimension: nt)
Definition at line 106 of file rdata.h.
```

```
9.17.3.21 numstepsB
double* numstepsB
number of integration steps backward problem (dimension: nt)
Definition at line 109 of file rdata.h.
9.17.3.22 numrhsevals
double* numrhsevals
number of right hand side evaluations forward problem (dimension: nt)
Definition at line 112 of file rdata.h.
9.17.3.23 numrhsevalsB
double* numrhsevalsB
number of right hand side evaluations backwad problem (dimension: nt)
Definition at line 115 of file rdata.h.
9.17.3.24 numerrtestfails
double* numerrtestfails
number of error test failures forward problem (dimension: nt)
Definition at line 118 of file rdata.h.
9.17.3.25 numerrtestfailsB
double* numerrtestfailsB
number of error test failures backwad problem (dimension: nt)
Definition at line 121 of file rdata.h.
```

9.17.3.26 numnonlinsolvconvfails double* numnonlinsolvconvfails number of linear solver convergence failures forward problem (dimension: nt) Definition at line 125 of file rdata.h. 9.17.3.27 numnonlinsolvconvfailsB double* numnonlinsolvconvfailsB number of linear solver convergence failures backwad problem (dimension: nt) Definition at line 129 of file rdata.h. 9.17.3.28 order double* order employed order forward problem (dimension: nt) Definition at line 132 of file rdata.h. 9.17.3.29 newton status double* newton_status flag indicating success of Newton solver Definition at line 135 of file rdata.h. 9.17.3.30 newton_numsteps double* newton_numsteps number of Newton steps for steady state problem

Definition at line 141 of file rdata.h.

```
9.17.3.31 newton_numlinsteps
double* newton_numlinsteps
number of linear steps by Newton step for steady state problem
Definition at line 144 of file rdata.h.
9.17.3.32 xss
double* xss
steady state found be Newton solver
Definition at line 147 of file rdata.h.
9.17.3.33 IIh
double* 11h
likelihood value (double[1])
Definition at line 150 of file rdata.h.
9.17.3.34 chi2
double* chi2
chi2 value (double[1])
Definition at line 153 of file rdata.h.
9.17.3.35 sllh
double* sllh
parameter derivative of likelihood (dimension: nplist)
Definition at line 156 of file rdata.h.
```

```
9.17.3.36 s2llh
double* s211h
second order parameter derivative of likelihood (dimension: (nJ-1) x nplist, column-major)
Definition at line 160 of file rdata.h.
9.17.3.37 status
double* status
status code (double[1])
Definition at line 163 of file rdata.h.
9.17.3.38 np
const int np
total number of model parameters
Definition at line 210 of file rdata.h.
9.17.3.39 nk
const int nk
number of fixed parameters
Definition at line 212 of file rdata.h.
9.17.3.40 nx
const int nx
number of states
Definition at line 214 of file rdata.h.
```

```
9.17.3.41 nxtrue
const int nxtrue
number of states in the unaugmented system
Definition at line 216 of file rdata.h.
9.17.3.42 ny
const int ny
number of observables
Definition at line 218 of file rdata.h.
9.17.3.43 nytrue
const int nytrue
number of observables in the unaugmented system
Definition at line 220 of file rdata.h.
9.17.3.44 nz
const int nz
number of event outputs
Definition at line 222 of file rdata.h.
9.17.3.45 nztrue
const int nztrue
number of event outputs in the unaugmented system
Definition at line 224 of file rdata.h.
```

```
9.17.3.46 ne
const int ne
number of events
Definition at line 226 of file rdata.h.
9.17.3.47 nJ
const int nJ
dimension of the augmented objective function for 2nd order ASA
Definition at line 228 of file rdata.h.
9.17.3.48 nplist
const int nplist
number of parameter for which sensitivities were requested
Definition at line 231 of file rdata.h.
9.17.3.49 nmaxevent
const int nmaxevent
maximal number of occuring events (for every event type)
Definition at line 233 of file rdata.h.
9.17.3.50 nt
const int nt
number of considered timepoints
Definition at line 235 of file rdata.h.
```

```
9.17.3.51 newton_maxsteps
const int newton_maxsteps
maximal number of newton iterations for steady state calculation
Definition at line 237 of file rdata.h.
9.17.3.52 pscale
const AMICI_parameter_scaling pscale
scaling of parameterization (lin,log,log10)
Definition at line 239 of file rdata.h.
9.17.3.53 o2mode
const AMICI_o2mode o2mode
flag indicating whether second order sensitivities were requested
Definition at line 241 of file rdata.h.
9.17.3.54 sensi
const AMICI_sensi_order sensi
sensitivity order
Definition at line 243 of file rdata.h.
9.17.3.55 sensi_meth
const AMICI_sensi_meth sensi_meth
sensitivity method
```

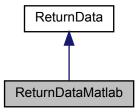
Definition at line 245 of file rdata.h.

9.18 ReturnDataMatlab Class Reference

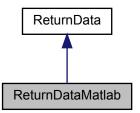
The ReturnDataMatlab class sets up ReturnData to be returned by the MATLAB mex functions. Memory is allocated using matlab functions.

```
#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 Member Function Documentation

9.18.2.1 initField2()

@ brief initialise matrix and attach to the field @ param FIELD name of the field to which the matrix will be attached @ param D1 number of rows in the matrix @ param D2 number of columns in the matrix

Reimplemented from ReturnData.

Definition at line 68 of file returndata_matlab.cpp.

9.18.2.2 initField3()

@ brief initialise 3D tensor and attach to the field @ param FIELD name of the field to which the tensor will be attached @ param D1 number of rows in the tensor @ param D2 number of columns in the tensor @ param D3 number of elements in the third dimension of the tensor

Reimplemented from ReturnData.

Definition at line 79 of file returndata_matlab.cpp.

9.18.2.3 initField4()

@ brief initialise 4D tensor and attach to the field @ param FIELD name of the field to which the tensor will be attached @ param D1 number of rows in the tensor @ param D2 number of columns in the tensor @ param D3 number of elements in the third dimension of the tensor @ param D4 number of elements in the fourth dimension of the tensor

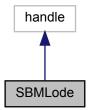
Reimplemented from ReturnData.

Definition at line 91 of file returndata_matlab.cpp.

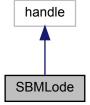
9.19 SBMLode Class Reference

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("")

conditior

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()

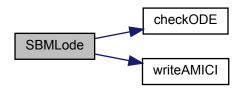
```
SBMLode ( {\tt matlabtypesubstitute} \  \, \textit{filename} \ )
```

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()

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
```

Definition at line 84 of file SBMLode.m.

compartment = sym.empty("")

Default: sym.empty("")

```
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.

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```
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
```

Definition at line 164 of file SBMLode.m.

funmath = cell.empty("")

Default: cell.empty("")

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()

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

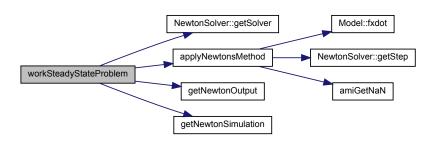
solver uses forward intergration, if the Newton solver fails

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

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()

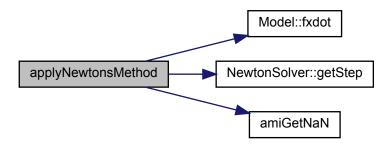
applyNewtonsMethod applies Newtons method to the current state \boldsymbol{x} to

find the steady state

@param[in] udata pointer to the user data struct
Type: UserData
@param[in] tdata pointer to the temporary data struct
Type: TempData
@param[out] tdata pointer to the temporary data struct
Type: TempData
@param[out] rdata pointer to the return data struct
Type: ReturnData
@param[in] newton_try integer for the try number of the Newton solver
@return void

Definition at line 83 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()

Newton solver

Parameters

```
in run_time | double computation time of the Newton solver
```

Returns

int status flag indicating success of execution

Type: int

Definition at line 237 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]
```

 ${\tt getNewtonSimulation}\ \, {\tt solves}\ \, {\tt the}\ \, {\tt forward}\ \, {\tt problem,}\ \, {\tt if}\ \, {\tt the}\ \, {\tt first}\ \, {\tt Newton}$

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 int status flag indicating success of execution <br><b>Type</b>: int
```

Definition at line 279 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

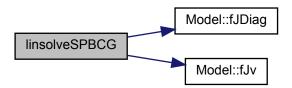
Returns

int status flag indicating success of execution

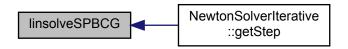
Type: int

Definition at line 346 of file steadystateproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

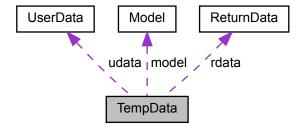


9.21 TempData Class Reference

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
- DIsMat Jtmp
- realtype * IIhS0
- realtype * Jy
- realtype * dJydp
- realtype * dJydy
- realtype * dJydsigma
- realtype * dJydx
- realtype * Jz
- realtype * dJzdp
- realtype * dJzdx
- realtype * dJzdz
- $\bullet \ \ realtype * \textbf{dJzdsigma}$
- 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 SIsMat 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 Member Data Documentation 9.21.2.1 p realtype* p = nullptr

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parameter array, unscaled

Definition at line 27 of file tdata.h.

9.21.2.2 t
realtype t
current time
Definition at line 30 of file tdata.h.
9.21.2.3 x
N_Vector x
state vector
Definition at line 33 of file tdata.h.
9.21.2.4 x_old
N_Vector x_old
old state vector
Definition at line 35 of file tdata.h.
9.21.2.5 x_disc
N_Vector* x_disc
array of state vectors at discontinuities
Definition at line 37 of file tdata.h.
9.21.2.6 xdot_disc
N_Vector* xdot_disc
array of differential state vectors at discontinuities
Definition at line 39 of file tdata.h.

```
9.21.2.7 xdot_old_disc
N_Vector* xdot_old_disc
array of old differential state vectors at discontinuities
Definition at line 41 of file tdata.h.
9.21.2.8 dx
N\_Vector\ dx
differential state vector
Definition at line 43 of file tdata.h.
9.21.2.9 dx_old
N_Vector dx_old
old differential state vector
Definition at line 45 of file tdata.h.
9.21.2.10 xdot
N_Vector xdot
time derivative state vector
Definition at line 47 of file tdata.h.
9.21.2.11 xdot_old
N_Vector xdot_old
old time derivative state vector
Definition at line 49 of file tdata.h.
```

9.21.2.12 xB
N_Vector xB
adjoint state vector
Definition at line 51 of file tdata.h.
9.21.2.13 xB_old
N_Vector xB_old
old adjoint state vector
Definition at line 53 of file tdata.h.
9.21.2.14 dxB
N_Vector dxB
differential adjoint state vector
Definition at line 55 of file tdata.h.
9.21.2.15 xQB
N_Vector xQB
quadrature state vector
Definition at line 57 of file tdata.h.
9.21.2.16 xQB_old
N_Vector xQB_old
old quadrature state vector
Definition at line 59 of file tdata.h.

```
9.21.2.17 sx
N_Vector* sx
sensitivity state vector array
Definition at line 61 of file tdata.h.
9.21.2.18 sdx
N_Vector* sdx
differential sensitivity state vector array
Definition at line 63 of file tdata.h.
9.21.2.19 Jtmp
DlsMat Jtmp
Jacobian
Definition at line 65 of file tdata.h.
9.21.2.20 IIhS0
realtype* llhS0
parameter derivative of likelihood array
Definition at line 68 of file tdata.h.
9.21.2.21 Jy
realtype* Jy
data likelihood
Definition at line 70 of file tdata.h.
```

9.21.2.22 dJydp realtype* dJydp parameter derivative of data likelihood Definition at line 72 of file tdata.h. 9.21.2.23 dJydy realtype* dJydy observable derivative of data likelihood Definition at line 74 of file tdata.h. 9.21.2.24 dJydsigma realtype* dJydsigma observable sigma derivative of data likelihood Definition at line 76 of file tdata.h. 9.21.2.25 dJydx realtype* dJydx state derivative of data likelihood Definition at line 78 of file tdata.h. 9.21.2.26 Jz realtype* Jz event likelihood Definition at line 80 of file tdata.h.

```
9.21.2.27 dJzdp
realtype* dJzdp
parameter derivative of event likelihood
Definition at line 82 of file tdata.h.
9.21.2.28 dJzdx
realtype* dJzdx
state derivative of event likelihood
Definition at line 84 of file tdata.h.
9.21.2.29 dJzdz
realtype* dJzdz
event ouput derivative of event likelihood
Definition at line 86 of file tdata.h.
9.21.2.30 dJzdsigma
realtype* dJzdsigma
event sigma derivative of event likelihood
Definition at line 88 of file tdata.h.
9.21.2.31 dJrzdz
```

realtype* dJrzdz

event ouput derivative of event likelihood at final timepoint

Definition at line 90 of file tdata.h.

```
9.21.2.32 dJrzdsigma
realtype* dJrzdsigma
event sigma derivative of event likelihood at final timepoint
Definition at line 92 of file tdata.h.
9.21.2.33 dzdx
realtype* dzdx
state derivative of event output
Definition at line 94 of file tdata.h.
9.21.2.34 dzdp
realtype* dzdp
parameter derivative of event output
Definition at line 96 of file tdata.h.
9.21.2.35 drzdx
realtype* drzdx
state derivative of event timepoint
Definition at line 98 of file tdata.h.
9.21.2.36 drzdp
realtype* drzdp
parameter derivative of event timepoint
Definition at line 100 of file tdata.h.
```

```
9.21.2.37 dydp
realtype* dydp
parameter derivative of observable
Definition at line 102 of file tdata.h.
9.21.2.38 dydx
realtype* dydx
state derivative of observable
Definition at line 104 of file tdata.h.
9.21.2.39 yS0
realtype* yS0
initial sensitivity of observable
Definition at line 106 of file tdata.h.
9.21.2.40 sigmay
realtype* sigmay
data standard deviation
Definition at line 108 of file tdata.h.
9.21.2.41 dsigmaydp
realtype* dsigmaydp
parameter derivative of data standard deviation
```

Definition at line 110 of file tdata.h.

9.21.2.42 sigmaz realtype* sigmaz event standard deviation Definition at line 112 of file tdata.h. 9.21.2.43 dsigmazdp realtype* dsigmazdp parameter derivative of event standard deviation Definition at line 114 of file tdata.h. 9.21.2.44 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 121 of file tdata.h. 9.21.2.45 rootidx int* rootidx array of index which root has been found Definition at line 123 of file tdata.h. 9.21.2.46 nroots int* nroots array of number of found roots for a certain event type Definition at line 125 of file tdata.h.

```
9.21.2.47 rootvals
realtype* rootvals
array of values of the root function
Definition at line 127 of file tdata.h.
9.21.2.48 h
realtype* h
temporary rootval storage to check crossing in secondary event
Definition at line 129 of file tdata.h.
9.21.2.49 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 134 of file tdata.h.
9.21.2.50 deltax
realtype* deltax
change in x
Definition at line 137 of file tdata.h.
9.21.2.51 deltasx
realtype* deltasx
```

Definition at line 139 of file tdata.h.

change in sx

9.21.2.52 deltaxB realtype* deltaxB change in xB Definition at line 141 of file tdata.h. 9.21.2.53 deltaqB realtype* deltaqB change in qB Definition at line 143 of file tdata.h. 9.21.2.54 which int which integer for indexing of backwards problems Definition at line 146 of file tdata.h. 9.21.2.55 discs realtype* discs array containing the time-points of discontinuities Definition at line 149 of file tdata.h. 9.21.2.56 irdiscs realtype* irdiscs array containing the index of discontinuities Definition at line 151 of file tdata.h.

9.21.2.57 J

```
SlsMat J = NULL
```

tempory storage of Jacobian data across functions

Definition at line 154 of file tdata.h.

9.21.2.58 dxdotdp

```
realtype* dxdotdp = NULL
```

tempory storage of dxdotdp data across functions

Definition at line 156 of file tdata.h.

9.21.2.59 w

```
realtype* w = NULL
```

tempory storage of w data across functions

Definition at line 158 of file tdata.h.

9.21.2.60 dwdx

```
realtype* dwdx = NULL
```

tempory storage of dwdx data across functions

Definition at line 160 of file tdata.h.

9.21.2.61 dwdp

```
realtype* dwdp = NULL
```

tempory storage of dwdp data across functions

Definition at line 162 of file tdata.h.

```
9.21.2.62 M
realtype* M = NULL
tempory storage of M data across functions
Definition at line 164 of file tdata.h.
9.21.2.63 dfdx
realtype* dfdx = NULL
tempory storage of dfdx data across functions
Definition at line 166 of file tdata.h.
9.21.2.64 stau
realtype* stau = NULL
tempory storage of stau data across functions
Definition at line 168 of file tdata.h.
9.21.2.65 nplist
int nplist
number of parameters, copied from udata, necessary for deallocation
Definition at line 171 of file tdata.h.
9.21.2.66 iroot
```

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

int iroot = 0

Definition at line 175 of file tdata.h.

Generated by Doxygen

```
9.21.2.67 nan_dxdotdp
booleantype nan_dxdotdp = false
flag indicating whether a NaN in dxdotdp has been reported
Definition at line 178 of file tdata.h.
9.21.2.68 nan_J
booleantype nan_J = false
flag indicating whether a NaN in J has been reported
Definition at line 180 of file tdata.h.
9.21.2.69 nan_JDiag
booleantype nan_JDiag = false
flag indicating whether a NaN in JDiag has been reported
Definition at line 182 of file tdata.h.
9.21.2.70 nan_JSparse
booleantype nan_JSparse = false
flag indicating whether a NaN in JSparse has been reported
Definition at line 184 of file tdata.h.
```

9.21.2.71 nan_xdot

booleantype nan_xdot = false

flag indicating whether a NaN in xdot has been reported

Definition at line 186 of file tdata.h.

```
9.21.2.72 nan_xBdot
booleantype nan_xBdot = false
flag indicating whether a NaN in xBdot has been reported
Definition at line 188 of file tdata.h.
9.21.2.73 nan_qBdot
booleantype nan_qBdot = false
flag indicating whether a NaN in qBdot has been reported
Definition at line 190 of file tdata.h.
9.21.2.74 udata
const UserData* udata
attached UserData object
Definition at line 193 of file tdata.h.
9.21.2.75 model
Model* model
attached Model object
Definition at line 195 of file tdata.h.
9.21.2.76 rdata
ReturnData* rdata
attached ReturnData object
Definition at line 197 of file tdata.h.
9.21.2.77 solver
Solver* solver = nullptr
attached Solver object
```

Definition at line 199 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
- 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 Imm
- 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 print()
void print ( )
function to print the contents of the UserData object
Definition at line 84 of file udata.cpp.
9.22.3 Member Data Documentation
9.22.3.1 nmaxevent
int nmaxevent
maximal number of events to track
Definition at line 25 of file udata.h.
9.22.3.2 qpositivex
double* qpositivex
positivity flag
Definition at line 28 of file udata.h.
9.22.3.3 plist
int* plist
parameter selection and reordering
```

Definition at line 31 of file udata.h.

9.22.3.4 nplist
int nplist
number of parameters in plist
Definition at line 33 of file udata.h.
9.22.3.5 nt
int nt
number of timepoints
Definition at line 36 of file udata.h.
9.22.3.6 p
double* p
parameter array
Definition at line 39 of file udata.h.
9.22.3.7 k
double* k
constants array
Definition at line 42 of file udata.h.
9.22.3.8 pscale
AMICI_parameter_scaling pscale
parameter transformation of p
Definition at line 45 of file udata.h.

9.22.3.9 tstart
double tstart
starting time
Definition at line 48 of file udata.h.
9.22.3.10 ts
double* ts
timepoints
Definition at line 50 of file udata.h.
9.22.3.11 pbar
double* pbar
scaling of parameters
Definition at line 53 of file udata.h.
9.22.3.12 xbar
double* xbar
scaling of states
Definition at line 55 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 58 of file udata.h.

9.22.3.14 atol double atol absolute tolerances for integration Definition at line 60 of file udata.h. 9.22.3.15 rtol double rtol relative tolerances for integration Definition at line 62 of file udata.h. 9.22.3.16 maxsteps int maxsteps maximum number of allowed integration steps Definition at line 64 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 67 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 70 of file udata.h.

9.22.3.19 newton_preeq int newton_preeq Preequilibration of model via NEwton solver? Definition at line 72 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 75 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 82 of file udata.h. 9.22.3.22 sensi_meth AMICI_sensi_meth sensi_meth method for sensitivity computation Definition at line 85 of file udata.h. 9.22.3.23 linsol int linsol linear solver specification

Definition at line 88 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 96 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 103 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 110 of file udata.h.

9.22.3.27 stldet

booleantype stldet

flag controlling stability limit detection

Definition at line 113 of file udata.h.

9.22.3.28 x0data

double* x0data

state initialisation

Definition at line 116 of file udata.h.

9.22.3.29 sx0data

```
double* sx0data
```

sensitivity initialisation

Definition at line 119 of file udata.h.

9.22.3.30 ordering

```
int ordering
```

state ordering

Definition at line 122 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()

Parameters

varargin

```
amiwrap ( modelname, symfun, tdir, o2flag )
```

Required Parameters for varargin:

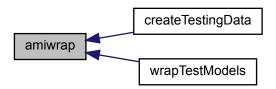
- modelname specifies the name of the model which will be later used for the naming of the simulation file
- symfun specifies a function which executes model definition see Model Definition for details
- tdir target directory where the simulation file should be placed **Default:** \$AMICIDIR/models/modelname
- 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()

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()

```
\label{local_model} $$ \mbox{mlhsInnerSubst}<:::*int > \mbox{computeBracketLevel (} $$ :::*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

Include dependency graph for amici.cpp:

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>
```



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 printErrMsgldAndTxt (const char *identifier, const char *msg,...)
- void printWarnMsgldAndTxt (const char *identifier, const char *msg,...)

Variables

- msgldAndTxtFp errMsgldAndTxt = &printErrMsgldAndTxt
- msgldAndTxtFp warnMsgldAndTxt = &printWarnMsgldAndTxt

10.4.1 Function Documentation

10.4.1.1 runAmiciSimulation()

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

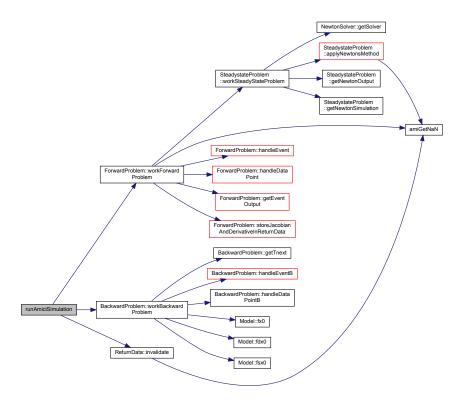
Returns

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 printErrMsgldAndTxt()

printErrMsgldAndTxt 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 printWarnMsgldAndTxt()

printErrMsgldAndTxt 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.

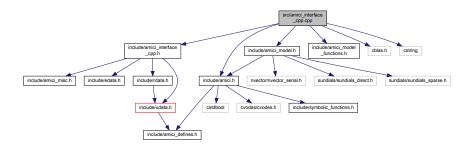
10.5 src/amici_interface_cpp.cpp File Reference

core routines for cpp interface

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

#include <cstring>

Include dependency graph for amici_interface_cpp.cpp:



Functions

- ReturnData * getSimulationResults (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()

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

Parameters

in	udata	pointer to user data object Type : UserData
in	edata	pointer to experimental data object Type : ExpData

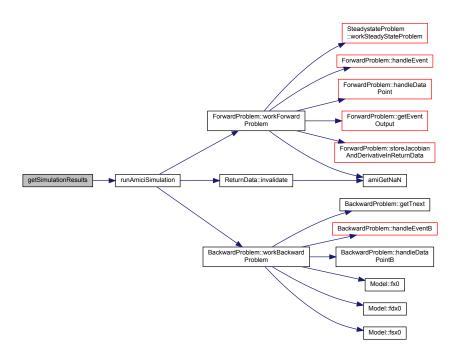
Returns

rdata pointer to return data object

Type: ReturnData

Definition at line 30 of file amici_interface_cpp.cpp.

Here is the call graph for this function:



10.5.1.2 amici_dgemm()

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

Parameters

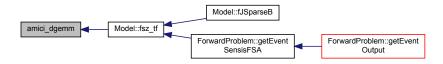
in	layout	can be AMICI_BLAS_ColMajor or AMICI_BLAS_RowMajor.
in	TransA	flag indicating whether A should be transposed before multiplication
in	TransB	flag indicating whether B should be transposed before multiplication
in	М	number of rows in A/C

Parameters

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	Α	matrix A
in	lda	leading dimension of A (m or k)
in	В	matrix B
in	ldb	leading dimension of B (k or n)
in	beta	coefficient beta
in,out	С	matrix C
in	ldc	leading dimension of C (m or n)

Definition at line 63 of file amici_interface_cpp.cpp.

Here is the caller graph for this function:



10.5.1.3 amici_dgemv()

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

Parameters

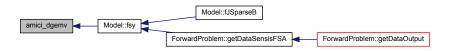
in	layout	can be AMICI_BLAS_ColMajor or AMICI_BLAS_RowMajor.
in	TransA	flag indicating whether A should be transposed before multiplication
in	М	number of rows in A
in	N	number of columns in A

Parameters

in	alpha	coefficient alpha
in	Α	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 86 of file amici_interface_cpp.cpp.

Here is the caller graph for this function:

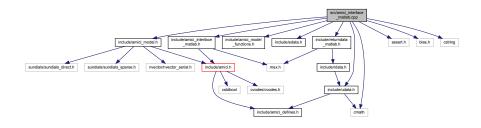


10.6 src/amici_interface_matlab.cpp File Reference

core routines for mex interface

```
#include "include/amici_interface_matlab.h"
#include "include/amici_model.h"
#include "include/amici_model_functions.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 K, const double alpha, const double *A, const int Ida, const double
 *B, const int Idb, const double beta, double *C, const int Idc)
- 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

Value:

@ 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 31 of file amici_interface_matlab.cpp.

10.6.2.2 readOptionData

Value:

@ brief extract information from a property of a matlab class (matrix) @ param OPTION name of the property Definition at line 44 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[] )
```

<<<<< HEAD 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.

mexFunction is the main function of the mex simulation file this function carries out all numerical integration and writes results into the sol struct.

master

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 71 of file amici_interface_matlab.cpp.

10.6.3.2 userDataFromMatlabCall()

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 122 of file amici_interface_matlab.cpp.

10.6.3.3 amici_blasCBlasTransToBlasTrans()

```
char amici_blasCBlasTransToBlasTrans ( {\tt 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

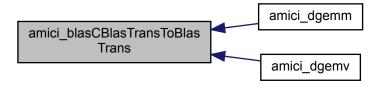
Returns

cblastrans CBlas readable CHAR indicating transposition and complex conjugation

Type: char

Definition at line 329 of file amici_interface_matlab.cpp.

Here is the caller graph for this function:



10.6.3.4 amici_dgemm()

amici_dgemm provides an interface to the CBlas 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	М	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	Α	matrix A
in	lda	leading dimension of A (m or k)
in	В	matrix B
in	ldb	leading dimension of B (k or n)
in	beta	coefficient beta
in,out	С	matrix C
in	ldc	leading dimension of C (m or n)

Returns

void

Definition at line 361 of file amici_interface_matlab.cpp.

Here is the call graph for this function:



10.6.3.5 amici_dgemv()

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	М	number of rows in A
in	N	number of columns in A
in	alpha	coefficient alpha
in	Α	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 404 of file amici_interface_matlab.cpp.

Here is the call graph for this function:



10.6.3.6 expDataFromMatlabCall()

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 432 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()

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 \geq = 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

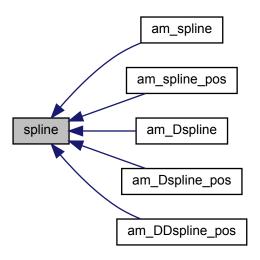
0	normal return	
1	less than two data points; cannot interpolate	
2	x[] are not in ascending order	

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()

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 \geq = 2)
in	и	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	С	array of spline coefficients computed by spline().
in	d	array of spline coefficients computed by spline().

Returns

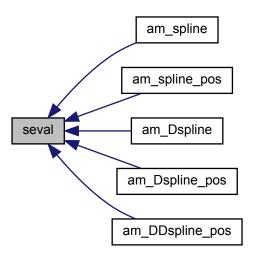
the value of the spline function at u

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()

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 \geq = 2)
in	и	the abscissa at which the spline is to be evaluated
in	x[]	the abscissas of the knots in strictly increasing order
in	у[]	the ordinates of the knots
in	b	array of spline coefficients computed by spline().
in	С	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.

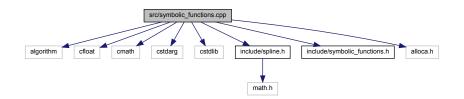
Definition at line 258 of file spline.cpp.

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 amilsNaN (double what)
- int amilsInf (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 amilsNaN()

c++ interface to the isNaN function

Parameters

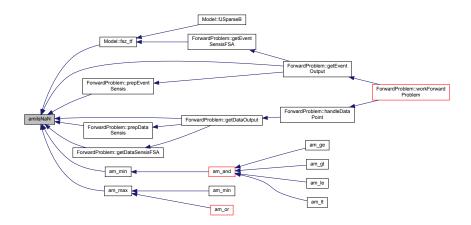
what argument

Returns

isnan(what)

Definition at line 32 of file symbolic_functions.cpp.

Here is the caller graph for this function:



10.8.2.2 amilsInf()

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 ( )
```

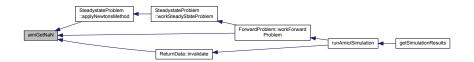
function returning nan

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 ( \mbox{double $x$ )} \label{eq: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 ( \mbox{double $x$} \ )
```

c implementation of matlab function heaviside

Parameters

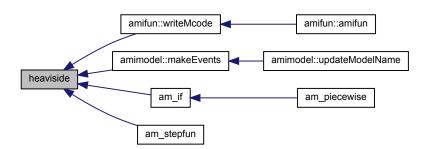
```
x argument
```

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

Χ	argument
---	----------

Returns

0

Type: double

Definition at line 110 of file symbolic_functions.cpp.

10.8.2.8 am_min()

```
double am_min ( \label{eq:condition} \mbox{double $a$,} \\ \mbox{double $c$ )}
```

c implementation of matlab function min

Parameters

а	value1
	Type: double
b	value2
	Type: double
С	bogus parameter to ensure correct parsing as a function
	Type: double

Returns

if (a < b) then a else b

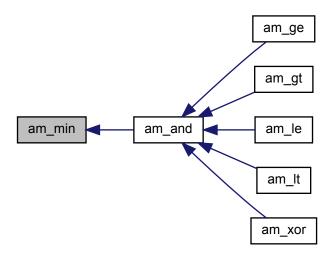
Type: double

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()

parameter derivative of c implementation of matlab function min

Parameters

id	argument index for differentiation	
а	value1	
	Type: double	
b	value2	
	Type: double	
С	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()

c implementation of matlab function max

Parameters

а	value1	
	Type: double	
b	value2	
	Type: double	
С	bogus parameter to ensure correct parsing as a function	
	Type: double	

Returns

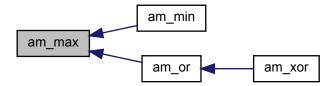
 $\label{eq:total_problem} \begin{tabular}{ll} \begin{tabular}{ll}$

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()

parameter derivative of c implementation of matlab function max

Parameters

id	argument index for differentiation	
а	value1	
	Type: double	
b	value2	
	Type: double	
С	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()

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

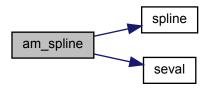
t	point at which the spline should be evaluated
num	number of spline nodes

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()

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

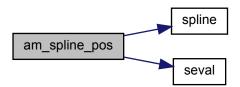
t point at which the spline should be num number of spline nodes		point at which the spline should be evaluated
		number of spline nodes

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

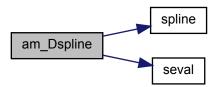
 id index of node to which the derivative of the corresponding spline coefficient should be of to point at which the spline should be evaluated num number of spline nodes 		index of node to which the derivative of the corresponding spline coefficient should be computed
		point at which the spline should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

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 \mathtt{dudt} user defined slope at first node. All arguments but id must be of type double.

Parameters

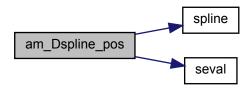
id	index of node to which the derivative of the corresponding spline coefficient should be computed
t point at which the spline should be evaluated	
num number of spline nodes	

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 compu	
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 \mathtt{dudt} user defined slope at first node. All arguments but id1 and id2 must be of type double.

Parameters

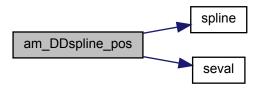
id1	index of node to which the first derivative of the corresponding spline coefficient should be computed	
id2	index of node to which the second derivative of the corresponding spline coefficient should be computed	
t	point at which the spline should be evaluated	
num	number of spline nodes	

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()

Parameters

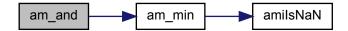
а	first input parameter
b	second input parameter

Return values

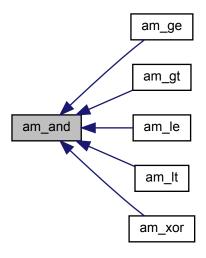
fun | logical value, negative for false, positive for true

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()

```
\label{lem:mather_mather} $$ mlhsInnerSubst< mathebypesubstitute > am_eq ($ mathebypesubstitute \ varargin ) $$
```

Parameters

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()

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()

Parameters

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

Return values

fun if condition is	rue 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 \leq 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()

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()

Parameters

а	first input parameter
b	second input parameter

Return values

fun	maximum of a and b
	maximum or 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()

Parameters

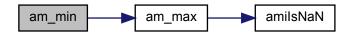
а	first input parameter
b	second input parameter

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

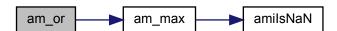
а	first input parameter
b	second input parameter

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()

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 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

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()
```

Parameters

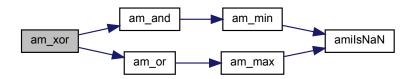
а	first input parameter
b	second input parameter

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