AMICI

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1 AMICI 0.1 General Documentation

1.1 Introduction

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

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

1.2 Availability

The sources for AMICI are accessible as

- Source tarball
- Source zipball
- GIT repository on github

Once you've obtained your copy check out the Installation

1.2.1 Obtaining AMICI via the GIT versioning system

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

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

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

1.2.2 License Conditions

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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 SBMLimporter

MATLAB toolbox to generate ODE models from SBML files

3 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.

3.1 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.

3.1.1 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()
```

3.1.2 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.

3.1.3 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 ];
```

3.1.4 Parameters

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

```
\verb"syms" param1" param2" param3" param4" param5" param6
```

Create the parameters vector

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

3.1 Model Definition 5

3.1.5 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];
```

3.1.6 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.

3.1.7 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];
```

3.1.8 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.

3.1.9 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

3.1.10 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.

3.1.11 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;
```

3.2 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()

3.3 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.

3.3.1 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.

3.3.2 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.

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3.3.3 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.

3.3.4 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.

4 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.

5 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.)

6 Hierarchical Index

6.1 Class Hierarchy

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

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optsym	126
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UserData	180
7 Class Index	
7.1 Class List	
Here are the classes, structs, unions and interfaces with brief descriptions:	
amidata AMIDATA provides a data container to pass experimental data to the simulation r likelihood computation. when any of the properties are updated, the class automatica consistency of dimension and updates related properties and initialises them with N	lly checks
amievent AMIEVENT defines events which later on will be transformed into appropriate C code	e 19
amifun AMIFUN defines functions which later on will be transformed into appropriate C code	e 22
amimodel AMIMODEL carries all model definitions including functions and events	33
amioption AMIOPTION provides an option container to pass simulation parameters to the simulation	lation rou- 56
amised AMISED is a container for SED-ML objects	65
BackwardProblem Class to solve backwards problems	69
ExpData Struct that carries all information about experimental data	75
ForwardProblem Groups all functions for solving the backwards problem. Has only static members	77
Model AMICI ODE model. The model does not contain any data, its state should never chan	ige 95
modelTest MODELTEST Summary of this class goes here Detailed explanation goes here	126
optsym OPTSYM is an auxiliary class to gain access to the private symbolic property s whi essary to be able to call symobj::optimize on it	ch is nec-
ReturnData Struct that stores all data which is later returned by the mex function	128
ReturnDataMatlab Sets up ReturnData to be returned by the MATLAB mex functions. Memory is alloca matlab functions	ated using

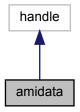
SBMLMODEL provides an intermediate container between the SBML definition and an ami- model object	145
Solver	
Solver class	152
SteadystateProblem	
Solves a steady-state problem using Newton's method and falls back to integration on failure	158
TempData	
Struct that provides temporary storage for different variables	163
UserData	
Struct that stores all user provided data	180

8 Class Documentation

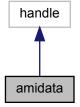
8.1 amidata Class Reference

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

8.1.1 Detailed Description

Definition at line 17 of file amidata.m.

8.1.2 Constructor & Destructor Documentation

```
8.1.2.1 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.
Definition at line 122 of the amidata.m.
8.1.3 Member Data Documentation
8.1.3.1 nt
nt = 0
Default: 0
Note
This property has custom functionality when its value is changed.
Definition at line 31 of file amidata.m.
0122 mg
8.1.3.2 ny
ny = 0
Default: 0
Nata
Note
This property has custom functionality when its value is changed.
Definition at line 39 of file amidata.m.
8.1.3.3 nz
nz = 0
Potentia 0
Default: 0
Note
This property has custom functionality when its value is changed.
Definition at line 47 of file amidata.m.

```
8.1.3.4 ne ne = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 55 of file amidata.m.

```
8.1.3.5 nk nk = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 63 of file amidata.m.

```
8.1.3.6 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.

```
8.1.3.7 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.

```
8.1.3.8 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.
8.1.3.9 Z
Z = double.empty("")
Default: double.empty("")
Note
     This property has custom functionality when its value is changed.
Definition at line 95 of file amidata.m.
8.1.3.10 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.
8.1.3.11 condition
condition = double.empty("")
Default: double.empty("")
```

Definition at line 111 of file amidata.m.

This property has custom functionality when its value is changed.

Note

8.2 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

8.2.1 Detailed Description

Definition at line 17 of file amievent.m.

8.2.2 Constructor & Destructor Documentation

8.2.2.1 amievent()

```
amievent (  \\ \text{matlabtypesubstitute } trigger, \\ \text{matlabtypesubstitute } bolus, \\ \text{matlabtypesubstitute } z \ ) \\
```

Parameters

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

Definition at line 75 of file amievent.m.

Here is the call graph for this function:



8.2.3 Member Function Documentation

8.2.3.1 setHflag()

Parameters

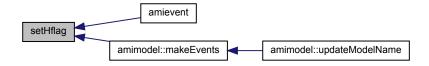
hflag	value for the hflag property
-------	------------------------------

Return values

this	updated event definition object
------	---------------------------------

Definition at line 18 of file setHflag.m.

Here is the caller graph for this function:



8.2.4 Member Data Documentation

```
8.2.4.1 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.

8.2.4.2 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.

8.2.4.3 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.

8.2.4.4 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.

8.3 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

mlhslnnerSubst< 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

8.3.1 Detailed Description

Definition at line 17 of file amifun.m.

8.3.2 Constructor & Destructor Documentation

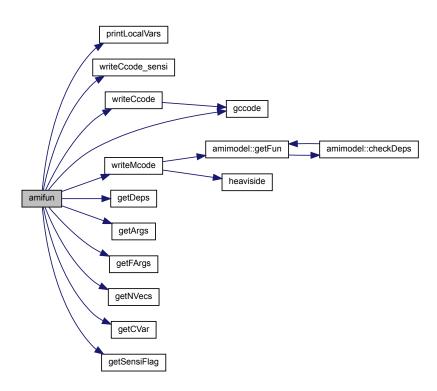
8.3.2.1 amifun()

Parameters

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

Definition at line 119 of file amifun.m.

Here is the call graph for this function:



8.3.3 Member Function Documentation

8.3.3.1 printLocalVars()

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

Parameters

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

Return values

fid	Nothing

Definition at line 18 of file printLocalVars.m.

Here is the caller graph for this function:



8.3.3.2 writeCcode_sensi()

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

Parameters

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

Return values



Definition at line 18 of file writeCcode_sensi.m.

Here is the caller graph for this function:



8.3.3.3 writeCcode()

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

Parameters

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

Return values



Definition at line 18 of file writeCcode.m.

Here is the call graph for this function:



Here is the caller graph for this function:



8.3.3.4 writeMcode()

Parameters

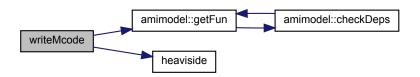
model	model defintion object
-------	------------------------

Return values

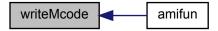
model	void

Definition at line 18 of file writeMcode.m.

Here is the call graph for this function:



Here is the caller graph for this function:



8.3.3.5 gccode()

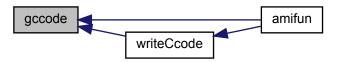
Parameters

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

Return values

Definition at line 18 of file gccode.m.

Here is the caller graph for this function:



8.3.3.6 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:



8.3.3.7 getArgs()

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:



8.3.3.8 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:



8.3.3.9 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:



8.3.3.10 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:



8.3.3.11 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:



8.3.4 Member Data Documentation

8.3.4.1 sym

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

Default: sym("[]")

Definition at line 27 of file amifun.m.

8.3.4.2 sym_noopt

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

Default: sym("[]")

Definition at line 35 of file amifun.m.

8.3.4.3 strsym

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

Default: sym("[]")

Definition at line 43 of file amifun.m.

```
8.3.4.4 strsym_old
strsym_old = sym("[]")
Default: sym("[]")
Definition at line 51 of file amifun.m.
8.3.4.5 funstr
funstr = char.empty("")
Default: char.empty("")
Definition at line 59 of file amifun.m.
8.3.4.6 cvar
cvar = char.empty("")
Default: char.empty("")
Definition at line 67 of file amifun.m.
8.3.4.7 argstr
argstr = char.empty("")
Default: char.empty("")
Definition at line 75 of file amifun.m.
8.3.4.8 fargstr
fargstr = char.empty("")
```

Default: char.empty("")

Definition at line 83 of file amifun.m.

8.3.4.9 deps

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

Default: cell.empty("")

Definition at line 91 of file amifun.m.

8.3.4.10 nvecs

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

Default: cell.empty("")

Definition at line 99 of file amifun.m.

8.3.4.11 sensiflag

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

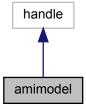
Default: logical.empty("")

Definition at line 107 of file amifun.m.

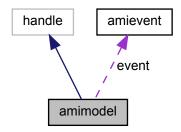
8.4 amimodel Class Reference

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

8.4.1 Detailed Description

Definition at line 17 of file amimodel.m.

8.4.2 Constructor & Destructor Documentation

8.4.2.1 amimodel()

Parameters

symfun	this is the string to the function which generates the modelstruct. You can also directly pass the struct here	
modelname	name of the model	1

Definition at line 526 of file amimodel.m.

Here is the caller graph for this function:



8.4.3 Member Function Documentation

8.4.3.1 updateRHS()

```
noret::substitute updateRHS ( {\tt matlabtypesubstitute} \  \  {\tt xdot} \ )
```

Parameters

xdot	new right hand side of the differential equation	
------	--	--

Definition at line 623 of file amimodel.m.

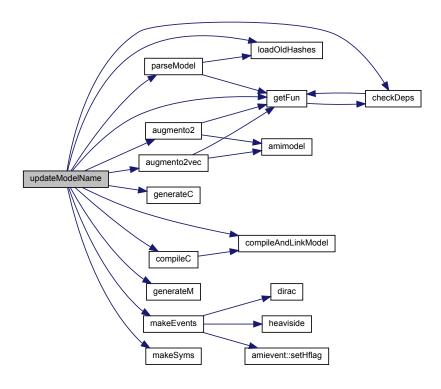
8.4.3.2 updateModelName()

Parameters

modelname	new modelname

Definition at line 636 of file amimodel.m.

Here is the call graph for this function:



8.4.3.3 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:



8.4.3.4 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:



8.4.3.5 generateM()

Parameters

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

Return values

this model definition object

Definition at line 18 of file generateM.m.

Here is the caller graph for this function:



8.4.3.6 getFun()

Parameters

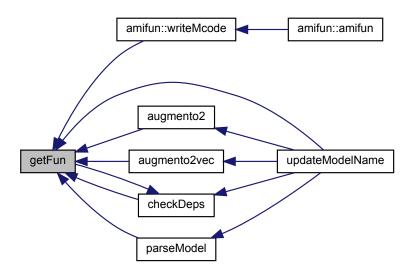
HTable	struct with hashes of symbolic definition from the previous compilation
funstr	function for which symbolic expressions should be computed

Definition at line 18 of file getFun.m.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.3.7 checkDeps()

Parameters

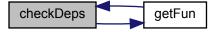
HTable	struct with reference hashes of functions in its fields
deps	cell array with containing a list of dependencies

Return values

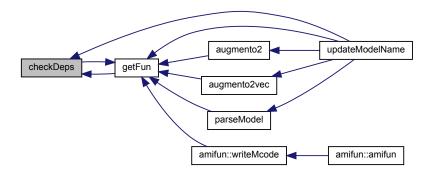
cflag	boolean indicating whether any of the dependencies have changed with respect to the hashes stored in	
	HTable	

Definition at line 18 of file checkDeps.m.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.3.8 loadOldHashes()

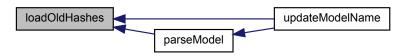
mlhsInnerSubst<::struct > loadOldHashes ()

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:



8.4.3.9 augmento2()

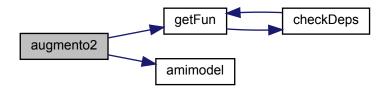
 $\verb|mlhsInnerSubst| < \verb|matlabtypesubstitute| > \verb|augmento2| ()$

Return values

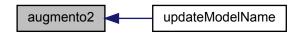
this augmented system which contains symbolic definition of the original system and its sensitivities

Definition at line 18 of file augmento2.m.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.3.10 augmento2vec()

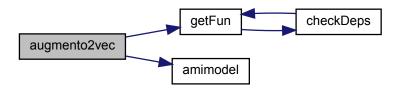
```
mlhsInnerSubst< matlabtypesubstitute > augmento2vec ( )
```

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:



8.4.3.11 compileAndLinkModel()

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

Parameters

modelname

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

Definition at line 18 of file compileAndLinkModel.m.

Here is the caller graph for this function:



8.4.4 Member Data Documentation

8.4.4.1 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.

8.4.4.2 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.

```
8.4.4.3 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.
8.4.4.4 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.
8.4.4.5 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.
8.4.4.6 debug
debug = false
Note
    This property has non-standard access specifiers: SetAccess = Private, GetAccess =
```

Definition at line 83 of file amimodel.m.

Default: false

Matlab documentation of property attributes.

```
8.4.4.7 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.

8.4.4.8 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.

8.4.4.9 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.

8.4.4.10 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.

```
8.4.4.11 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.
8.4.4.12 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.
8.4.4.13 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.
8.4.4.14 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.

```
8.4.4.15 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.
8.4.4.16 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.
8.4.4.17 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.
8.4.4.18 ng
ng = double.empty("")
```

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

Note

```
8.4.4.19 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.
8.4.4.20 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.
8.4.4.21 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.
8.4.4.22 id
id = double.empty("")
Note
    This property has non-standard access specifiers: SetAccess = Private, GetAccess =
    Public
    Matlab documentation of property attributes.
```

Definition at line 259 of file amimodel.m.

Default: double.empty("")

```
8.4.4.23 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.

```
8.4.4.24 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.

8.4.4.25 nnz

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

Note

This property has non-standard access specifiers: SetAccess = Private, GetAccess = Public

Matlab documentation of property attributes.

Default: double.empty("")

Definition at line 292 of file amimodel.m.

8.4.4.26 sparseidx

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

Note

This property has non-standard access specifiers: SetAccess = Private, GetAccess = Public

Matlab documentation of property attributes.

Default: double.empty("")

Definition at line 303 of file amimodel.m.

```
8.4.4.27 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.

8.4.4.28 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.

8.4.4.29 sparseidxB

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

Note

This property has non-standard access specifiers: SetAccess = Private, GetAccess = Public

Matlab documentation of property attributes.

Default: double.empty("")

Definition at line 336 of file amimodel.m.

8.4.4.30 rowvalsB

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

Note

This property has non-standard access specifiers: SetAccess = Private, GetAccess = Public

Matlab documentation of property attributes.

Default: double.empty("")

Definition at line 347 of file amimodel.m.

```
8.4.4.31 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.

8.4.4.32 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.

8.4.4.33 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.

8.4.4.34 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.

```
8.4.4.35 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.
8.4.4.36 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.
8.4.4.37 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.
8.4.4.38 cfun
cfun = struct.empty("")
Note
    This property has non-standard access specifiers: SetAccess = Private, GetAccess =
```

Definition at line 435 of file amimodel.m.

Default: struct.empty("")

Matlab documentation of property attributes.

8.4.4.39 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.

8.4.4.40 z2event

z2event = double.empty("")

Default: double.empty("")

Definition at line 466 of file amimodel.m.

8.4.4.41 splineflag

splineflag = false

Default: false

Definition at line 474 of file amimodel.m.

8.4.4.42 minflag

minflag = false

Default: false

Definition at line 482 of file amimodel.m.

8.4.4.43 maxflag

maxflag = false

Default: false

Definition at line 490 of file amimodel.m.

8.4.4.44 nw

nw = 0

Default: 0

Definition at line 498 of file amimodel.m.

8.4.4.45 ndwdx

ndwdx = 0

Default: 0

Definition at line 507 of file amimodel.m.

8.4.4.46 ndwdp

ndwdp = 0

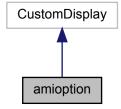
Default: 0

Definition at line 515 of file amimodel.m.

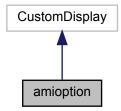
8.5 amioption Class Reference

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 linsol = 10
          newton solver: linear solver

    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 = 0
          preequilibration of system via newton solver (0 = none, 1 = only states, 2 = states and sensitivities)

    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
8.5.1 Detailed Description
Definition at line 17 of file amioption.m.
8.5.2 Constructor & Destructor Documentation
8.5.2.1 amioption()
amioption (
                {\tt matlabtypesubstitute}\ {\it varargin}\ )
OPTS = amioption(PARAM, VAL, ...) creates a set of options with the named parameters altered with the specified
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 283 of file amioption.m.

8.5.3 Member Data Documentation

```
8.5.3.1 atol
```

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

Default: 1e-16

Definition at line 28 of file amioption.m.

8.5.3.2 rtol

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

Default: 1e-8

Definition at line 36 of file amioption.m.

8.5.3.3 maxsteps

```
maxsteps = 1e4
```

Default: 1e4

Definition at line 44 of file amioption.m.

8.5.3.4 sens_ind

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

Default: double.empty("")

Definition at line 52 of file amioption.m.

8.5.3.5 qpositivex qpositivex = double.empty("") **Default:** double.empty("") Definition at line 60 of file amioption.m. 8.5.3.6 pbar pbar = double.empty("") **Default:** double.empty("") Definition at line 68 of file amioption.m. 8.5.3.7 tstart tstart = 0Default: 0 Definition at line 76 of file amioption.m. 8.5.3.8 lmm lmm = 2Default: 2 Definition at line 84 of file amioption.m. 8.5.3.9 iter iter = 2Default: 2

Definition at line 92 of file amioption.m.

8.5.3.10 linsol linsol = 9 Default: 9 Definition at line 100 of file amioption.m. 8.5.3.11 stldet stldet = true Default: true Definition at line 108 of file amioption.m. 8.5.3.12 interpType interpType = 1 Default: 1 Definition at line 116 of file amioption.m. 8.5.3.13 ImmB lmmB = 2Default: 2 Definition at line 124 of file amioption.m. 8.5.3.14 iterB

Default: 2

iterB = 2

Definition at line 132 of file amioption.m.

```
8.5.3.15 ism
ism = 1
Default: 1
Definition at line 140 of file amioption.m.
8.5.3.16 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.
8.5.3.17 sensi
sensi = 0
Default: 0
Note
      This property has custom functionality when its value is changed.
Definition at line 156 of file amioption.m.
8.5.3.18 nmaxevent
nmaxevent = 10
Default: 10
```

Definition at line 164 of file amioption.m.

8.5.3.19 ordering

```
ordering = 0
```

Default: 0

Definition at line 172 of file amioption.m.

8.5.3.20 ss

ss = 0

Default: 0

Definition at line 180 of file amioption.m.

```
8.5.3.21 x0
```

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

Default: double.empty("")

Definition at line 188 of file amioption.m.

8.5.3.22 sx0

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

Default: double.empty("")

Definition at line 196 of file amioption.m.

8.5.3.23 newton_linsol

```
newton_linsol = 10
```

Default: 10

Note

This property has custom functionality when its value is changed.

Definition at line 204 of file amioption.m.

8.5.3.24 newton_precon

```
newton_precon = 1
```

Default: 1

Note

This property has custom functionality when its value is changed.

Definition at line 212 of file amioption.m.

8.5.3.25 newton_maxsteps

```
newton_maxsteps = 40
```

Default: 40

Note

This property has custom functionality when its value is changed.

Definition at line 221 of file amioption.m.

8.5.3.26 newton_maxlinsteps

```
newton_maxlinsteps = 100
```

Default: 100

Note

This property has custom functionality when its value is changed.

Definition at line 229 of file amioption.m.

8.5.3.27 newton_preeq

```
newton\_preeq = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 237 of file amioption.m.

8.5.3.28 z2event

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

Default: double.empty("")

Definition at line 246 of file amioption.m.

8.5.3.29 pscale

```
pscale = ""
```

Default: ""

Note

This property has custom functionality when its value is changed.

Definition at line 254 of file amioption.m.

8.5.3.30 id

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

Note

This property has the MATLAB attribute Hidden set to true. Matlab documentation of property attributes.

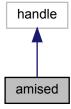
Default: double.empty("")

Definition at line 269 of file amioption.m.

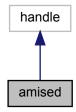
8.6 amised Class Reference

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

8.6.1 Detailed Description

Definition at line 17 of file amised.m.

8.6.2 Constructor & Destructor Documentation

8.6.2.1 amised()

```
amised ( {\tt matlabtypesubstitute}\ \ sedname\ )
```

Parameters

sedname	name/path of the SEDML document
---------	---------------------------------

Definition at line 112 of file amised.m.

Here is the call graph for this function:



8.6.3 Member Data Documentation

8.6.3.1 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.

8.6.3.2 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.

```
8.6.3.3 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.
8.6.3.4 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.
8.6.3.5 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.
8.6.3.6 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.

8.6.3.7 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.

8.7 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)

8.7.1 Detailed Description

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

Definition at line 19 of file backwardproblem.h.

8.7.2 Member Function Documentation

8.7.2.1 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

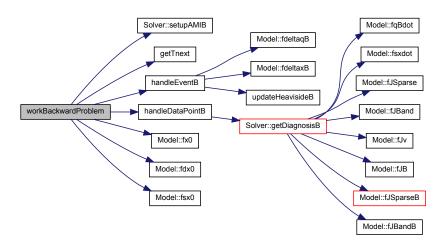
in	udata	pointer to the user data struct
		Type: UserData
in	tdata	pointer to the temporary data struct
		Type: TempData
out	rdata	pointer to the return data struct
		Type: ReturnData
in	model	pointer to model specification object
		Type: Model

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:



8.7.2.2 handleEventB()

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

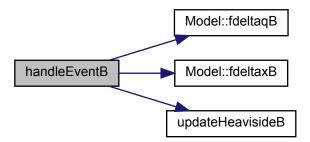
Returns

status flag indicating success of execution

Type: int

Definition at line 151 of file backwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.7.2.3 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

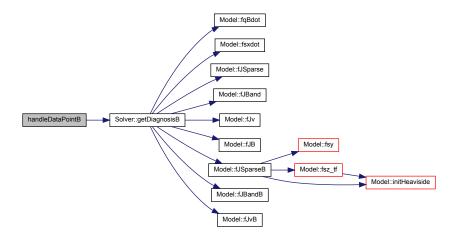
Returns

status flag indicating success of execution

Type: int

Definition at line 209 of file backwardproblem.cpp.

Here is the call graph for this function:





8.7.2.4 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 236 of file backwardproblem.cpp.

Here is the caller graph for this function:



8.7.2.5 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 260 of file backwardproblem.cpp.

Here is the caller graph for this function:



8.8 ExpData Class Reference

struct that carries all information about experimental data

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

Public Member Functions

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

Public Attributes

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

8.8.1 Detailed Description

Definition at line 8 of file edata.h.

8.8.2 Constructor & Destructor Documentation

8.8.2.1 ExpData() [1/2]

ExpData ()

default constructor

Definition at line 7 of file edata.cpp.



8.8.2.2 ExpData() [2/2]

initialization with UserData and model

Definition at line 11 of file edata.cpp.

Here is the call graph for this function:



8.8.3 Member Function Documentation

8.8.3.1 setDefaults()

```
void setDefaults ( )
```

initialization with default values

Definition at line 22 of file edata.cpp.

Here is the caller graph for this function:



8.8.4 Member Data Documentation

```
8.8.4.1 my
double* my
observed data
Definition at line 21 of file edata.h.
8.8.4.2 sigmay
double* sigmay
standard deviation of observed data
Definition at line 23 of file edata.h.
8.8.4.3 mz
double* mz
observed events
Definition at line 26 of file edata.h.
8.8.4.4 mrz
double* mrz
observed roots
Definition at line 28 of file edata.h.
8.8.4.5 sigmaz
double* sigmaz
standard deviation of observed events/roots
Definition at line 30 of file edata.h.
```

8.9 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)

8.9.1 Detailed Description

Definition at line 17 of file forwardproblem.h.

8.9.2 Member Function Documentation

8.9.2.1 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

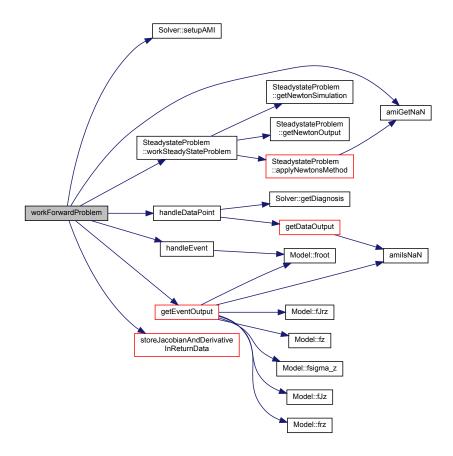
Returns

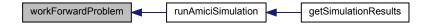
int status flag indicating success of execution

Type: int

Definition at line 11 of file forwardproblem.cpp.

Here is the call graph for this function:





8.9.2.2 handleEvent()

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

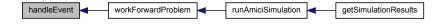
status flag indicating success of execution

Type: int

Definition at line 107 of file forwardproblem.cpp.



Here is the caller graph for this function:



8.9.2.3 storeJacobianAndDerivativeInReturnData()

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

Parameters

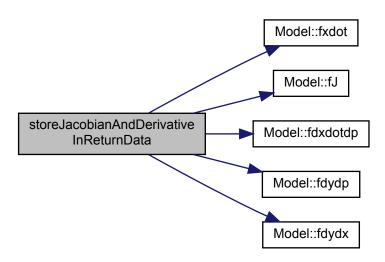
out	tdata	pointer to the temporary data struct Type : TempData
out	rdata	pointer to the return data struct Type : ReturnData
in	model	pointer to model specification object Type : Model

Returns

void

Definition at line 267 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:

```
storeJacobianAndDerivative uorkForwardProblem runAmiciSimulation getSimulationResults
```

8.9.2.4 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

Generated by Doxygen

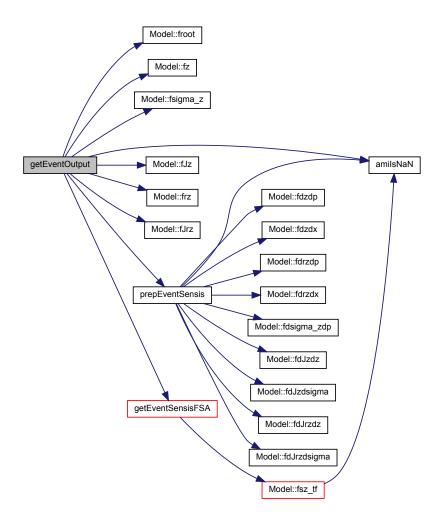
Returns

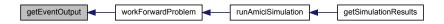
status flag indicating success of execution

Type: int

Definition at line 327 of file forwardproblem.cpp.

Here is the call graph for this function:





8.9.2.5 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

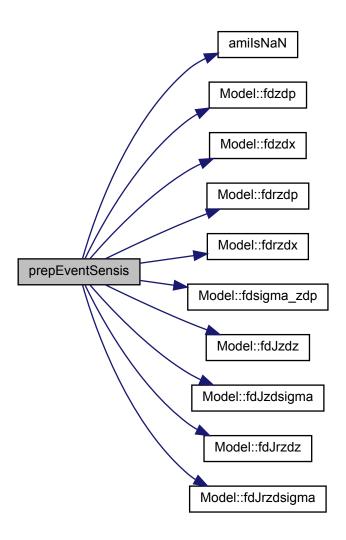
Returns

status flag indicating success of execution

 $\textbf{Type} \colon \mathsf{int}$

Definition at line 400 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.9.2.6 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

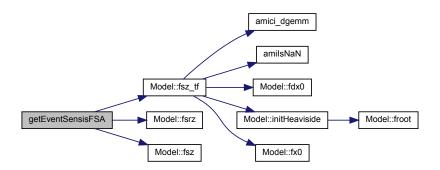
Returns

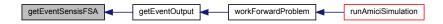
status flag indicating success of execution

Type: int

Definition at line 487 of file forwardproblem.cpp.

Here is the call graph for this function:





8.9.2.7 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

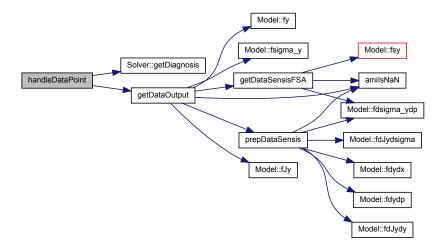
Returns

status flag indicating success of execution

Type: int

Definition at line 524 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.9.2.8 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

	1	
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

Parameters

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

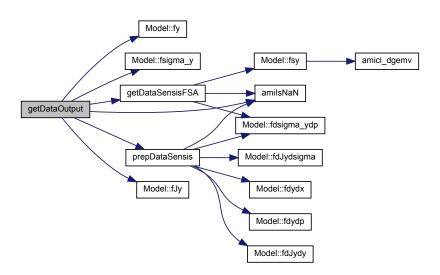
Returns

status flag indicating success of execution

Type: int

Definition at line 560 of file forwardproblem.cpp.

Here is the call graph for this function:





8.9.2.9 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

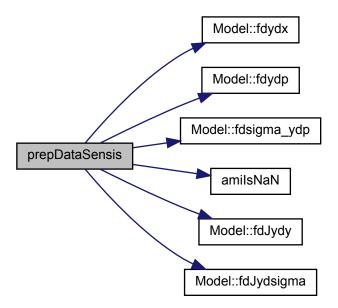
Returns

status flag indicating success of execution

Type: int

Definition at line 613 of file forwardproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.9.2.10 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

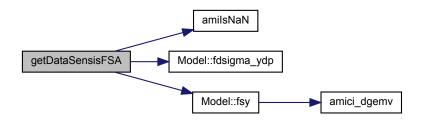
out	status	flag indicating success of execution Type : int
in	it	index of current timepoint Type: int
in	udata	pointer to the user data struct Type : UserData
out	rdata	pointer to the return data struct Type : ReturnData
in	edata	pointer to the experimental data struct Type : ExpData
out	tdata	pointer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

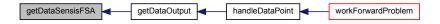
Returns

void

Definition at line 683 of file forwardproblem.cpp.

Here is the call graph for this function:





8.9.2.11 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 749 of file forwardproblem.cpp.

Here is the call graph for this function:



8.9.2.12 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 782 of file forwardproblem.cpp.

Here is the call graph for this function:



8.9.2.13 updateHeaviside()

updateHeaviside updates the heaviside variables h on event occurences

Parameters



Definition at line 817 of file forwardproblem.cpp.

8.10 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

8.10.1 Detailed Description

Definition at line 16 of file amici_model.h.

8.10.2 Member Function Documentation

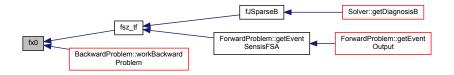
8.10.2.1 fx0()

```
virtual int fx0 (  \begin{tabular}{ll} N\_Vector & x0, \\ void * user\_data \end{tabular} \begin{tabular}{ll} (virtual) \end{tabular}
```

Initial states

Definition at line 52 of file amici_model.h.

Here is the caller graph for this function:



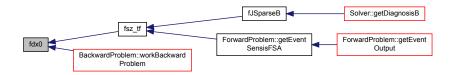
8.10.2.2 fdx0()

```
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 55 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.3 fsx0()

```
virtual int fsx0 (  & \text{N\_Vector} * sx0, \\ & \text{N\_Vector} x, \\ & \text{N\_Vector} dx, \\ & \text{void} * user\_data ) \quad [\text{virtual}]
```

Initial value for time derivative of states

Definition at line 60 of file amici_model.h.



8.10.2.4 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 63 of file amici_model.h.

8.10.2.5 fJ()

Jacobian of xdot with respect to states x

Definition at line 66 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.6 fJB()

```
virtual int fJB (

long int NeqBdot,
realtype t,
N_Vector x,
N_Vector xB,
N_Vector xBdot,
DlsMat JB,
void * user_data,
N_Vector tmplB,
```

```
N_Vector tmp2B,
N_Vector tmp3B ) [virtual]
```

Jacobian of xBdot with respect to adjoint state xB

Definition at line 69 of file amici_model.h.

Here is the caller graph for this function:

```
Solver::getDiagnosisB BackwardProblem::handleData PointB BackwardProblem::workBackward Problem
```

8.10.2.7 fJDiag()

diagonalized Jacobian (for preconditioning)

Definition at line 72 of file amici_model.h.

Here is the caller graph for this function:

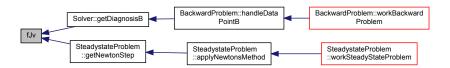


8.10.2.8 fJv()

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

Definition at line 75 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.9 froot()

Event trigger function for events

Definition at line 78 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.10 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 81 of file amici_model.h.



8.10.2.11 fsrz()

Sensitivity of rz, total derivative

Definition at line 84 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.12 fstau()

Sensitivity of event timepoint, total derivative

Definition at line 87 of file amici_model.h.

8.10.2.13 fy()

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

Observables / measurements

Definition at line 90 of file amici_model.h.



8.10.2.14 fdydp()

```
virtual int fdydp (  real type \ t, \\ int \ it, \\ N\_Vector \ x, \\ TempData * tdata ) \ [virtual]
```

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

Definition at line 93 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.15 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 96 of file amici_model.h.



8.10.2.16 fz()

Event-resolved measurements

Definition at line 99 of file amici_model.h.

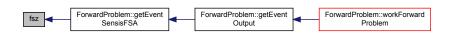
Here is the caller graph for this function:



8.10.2.17 fsz()

Sensitivity of z, total derivative

Definition at line 102 of file amici_model.h.



8.10.2.18 fdzdp()

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

Definition at line 105 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.19 fdzdx()

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

Definition at line 108 of file amici_model.h.



8.10.2.20 fdrzdp()

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

Definition at line 111 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.21 fdrzdx()

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

Definition at line 114 of file amici_model.h.



8.10.2.22 fxdot()

Right hand side of differential equation for states x

Definition at line 117 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.23 fxBdot()

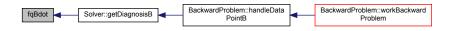
Right hand side of differential equation for adjoint state xB

Definition at line 120 of file amici_model.h.

8.10.2.24 fqBdot()

Right hand side of integral equation for quadrature states qB

Definition at line 123 of file amici_model.h.



8.10.2.25 fdxdotdp()

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

Definition at line 126 of file amici_model.h.

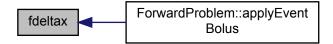
Here is the caller graph for this function:



8.10.2.26 fdeltax()

State update functions for events

Definition at line 129 of file amici_model.h.



8.10.2.27 fdeltasx()

Sensitivity update functions for events, total derivative

Definition at line 132 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.28 fdeltaxB()

Adjoint state update functions for events

Definition at line 135 of file amici_model.h.



8.10.2.29 fdeltaqB()

Quadrature state update functions for events

Definition at line 138 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.30 fsigma_y()

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

Standard deviation of measurements

Definition at line 141 of file amici_model.h.

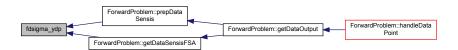


8.10.2.31 fdsigma_ydp()

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

Definition at line 144 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.32 fsigma_z()

Standard deviation of events

Definition at line 147 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.33 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 150 of file amici model.h.



8.10.2.34 fJy()

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

negative log-likelihood of time-resolved measurements y

Definition at line 153 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.35 fJz()

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

Definition at line 156 of file amici_model.h.



8.10.2.36 fJrz()

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

Definition at line 159 of file amici_model.h.

Here is the caller graph for this function:

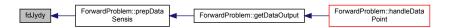


8.10.2.37 fdJydy()

```
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 162 of file amici_model.h.



8.10.2.38 fdJydsigma()

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

Definition at line 165 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.39 fdJzdz()

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

Definition at line 168 of file amici_model.h.



8.10.2.40 fdJzdsigma()

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

Definition at line 171 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.41 fdJrzdz()

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

Definition at line 174 of file amici_model.h.



8.10.2.42 fdJrzdsigma()

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

Definition at line 177 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.43 fsxdot()

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

Right hand side of differential equation for state sensitivities sx

Definition at line 180 of file amici_model.h.

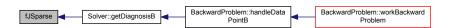


8.10.2.44 fJSparse()

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

Definition at line 183 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.45 fJBand()

J in banded form (for banded solvers)

Definition at line 186 of file amici_model.h.



8.10.2.46 fJBandB()

JB in banded form (for banded solvers)

Definition at line 189 of file amici_model.h.

Here is the caller graph for this function:



8.10.2.47 fJvB()

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

Definition at line 192 of file amici_model.h.

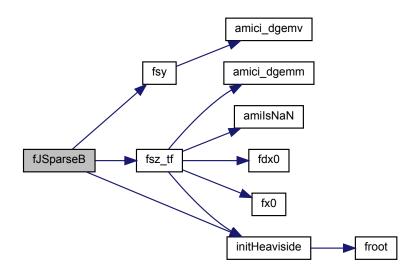


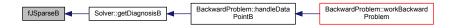
8.10.2.48 fJSparseB()

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

Definition at line 195 of file amici_model.h.

Here is the call graph for this function:





8.10.2.49 fsy()

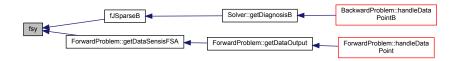
Sensitivity of measurements y, total derivative

Definition at line 25 of file amici_model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



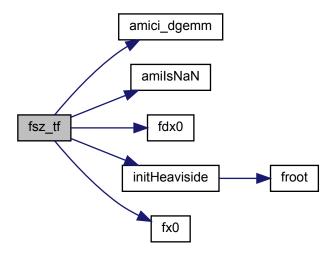
```
8.10.2.50 fsz_tf()
```

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

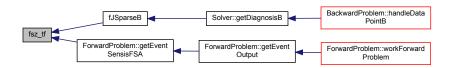
Sensitivity of z at final timepoint (ignores sensitivity of timepoint), total derivative

Definition at line 47 of file amici_model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.10.2.51 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

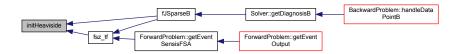
Type: int

Definition at line 409 of file amici_model.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.10.3 Member Data Documentation

8.10.3.1 np

const int np

total number of model parameters

Definition at line 235 of file amici_model.h.

8.10.3.2 nk

const int nk

number of fixed parameters

Definition at line 237 of file amici_model.h.

```
8.10.3.3 nx
const int nx
number of states
Definition at line 239 of file amici_model.h.
8.10.3.4 nxtrue
const int nxtrue
number of states in the unaugmented system
Definition at line 241 of file amici_model.h.
8.10.3.5 ny
const int ny
number of observables
Definition at line 243 of file amici_model.h.
8.10.3.6 nytrue
const int nytrue
number of observables in the unaugmented system
Definition at line 245 of file amici_model.h.
8.10.3.7 nz
const int nz
number of event outputs
Definition at line 247 of file amici_model.h.
```

```
8.10.3.8 nztrue
const int nztrue
number of event outputs in the unaugmented system
Definition at line 249 of file amici_model.h.
8.10.3.9 ne
const int ne
number of events
Definition at line 251 of file amici_model.h.
8.10.3.10 nw
const int nw
number of common expressions
Definition at line 253 of file amici_model.h.
8.10.3.11 ndwdx
const int ndwdx
number of derivatives of common expressions wrt x
Definition at line 255 of file amici_model.h.
8.10.3.12 ndwdp
const int ndwdp
number of derivatives of common expressions wrt p
Definition at line 257 of file amici_model.h.
```

```
8.10.3.13 nnz
const int nnz
number of nonzero entries in jacobian
Definition at line 259 of file amici_model.h.
8.10.3.14 nJ
const int nJ
dimension of the augmented objective function for 2nd order ASA
Definition at line 261 of file amici_model.h.
8.10.3.15 ubw
const int ubw
upper bandwith of the jacobian
Definition at line 263 of file amici_model.h.
8.10.3.16 lbw
const int lbw
lower bandwith of the jacobian
Definition at line 265 of file amici_model.h.
8.10.3.17 o2mode
const AMICI_o2mode o2mode
flag indicating whether for sensi == AMICI_SENSI_ORDER_SECOND directional or full second order derivative will
```

Definition at line 267 of file amici_model.h.

be computed

8.10.3.18 z2event

```
int* z2event = nullptr
```

index indicating to which event an event output belongs

Definition at line 269 of file amici_model.h.

8.10.3.19 idlist

```
realtype* idlist = nullptr
```

flag array for DAE equations

Definition at line 271 of file amici_model.h.

8.11 modelTest Class Reference

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

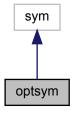
8.11.1 Detailed Description

Definition at line 17 of file modelTest.m.

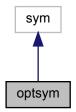
8.12 optsym Class Reference

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

Inheritance diagram for optsym:



Collaboration diagram for optsym:



Public Member Functions

- optsym (::sym symbol)
 optsym converts the symbolic object into a optsym object
- mlhsInnerSubst<::sym > getoptimized ()
 getoptimized calls symobj::optimize on the optsym object

8.12.1 Detailed Description

Definition at line 17 of file optsym.m.

8.12.2 Constructor & Destructor Documentation

8.12.2.1 optsym()

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

Parameters

symbol sy	mbolic object
-----------	---------------

Definition at line 32 of file optsym.m.

8.12.3 Member Function Documentation

8.12.3.1 getoptimized()

```
\verb|mlhsInnerSubst<::sym| > \verb|getoptimized| ( )
```

Return values

out optimized symbolic object

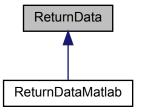
Definition at line 42 of file optsym.m.

8.13 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 nxconst int nxtrue
- const int ny
- const int nytrue
- . Constint hytruc
- 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

8.13.1 Detailed Description

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

Definition at line 11 of file rdata.h.

8.13.2 Member Function Documentation

8.13.2.1 invalidate()

void invalidate ()

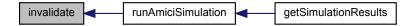
Parameters

in	udata	pointer to the user data struct
		Type: UserData

Definition at line 41 of file rdata.cpp.

Here is the call graph for this function:





8.13.2.2 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 349 of file rdata.cpp.

8.13.2.3 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 355 of file rdata.cpp.

8.13.2.4 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 360 of file rdata.cpp.

8.13.3 Member Data Documentation

Definition at line 46 of file rdata.h.

```
8.13.3.1 ts
double* ts
timepoints (dimension: nt)
Definition at line 34 of file rdata.h.
8.13.3.2 xdot
double* xdot
time derivative (dimension: nx)
Definition at line 37 of file rdata.h.
8.13.3.3 dxdotdp
double* dxdotdp
parameter derivative of time derivative (dimension: nx x nplist, column-major)
Definition at line 40 of file rdata.h.
8.13.3.4 dydx
double* dydx
state derivative of observables (dimension: ny x nx, column-major)
Definition at line 43 of file rdata.h.
8.13.3.5 dydp
double* dydp
parameter derivative of observables (dimension: ny x nplist, column-major)
```

```
8.13.3.6 J
double* J
Jacobian of differential equation right hand side (dimension: nx x nx, column-major)
Definition at line 49 of file rdata.h.
8.13.3.7 z
double* z
event output (dimension: nmaxevent x nz, column-major)
Definition at line 52 of file rdata.h.
8.13.3.8 sigmaz
double* sigmaz
event output sigma standard deviation (dimension: nmaxevent x nz, column-major)
Definition at line 55 of file rdata.h.
8.13.3.9 sz
double* sz
parameter derivative of event output (dimension: nmaxevent x nz, column-major)
Definition at line 58 of file rdata.h.
8.13.3.10 ssigmaz
double* ssigmaz
parameter derivative of event output standard deviation (dimension: nmaxevent x nz, column-major)
Definition at line 61 of file rdata.h.
```

```
8.13.3.11 rz
double* rz
event trigger output (dimension: nmaxevent x nz, column-major)
Definition at line 64 of file rdata.h.
8.13.3.12 srz
double* srz
parameter derivative of event trigger output (dimension: nmaxevent x nz x nplist, column-major)
Definition at line 67 of file rdata.h.
8.13.3.13 s2rz
double* s2rz
second order parameter derivative of event trigger output (dimension: nmaxevent x nztrue x nplist x nplist, column-
major)
Definition at line 70 of file rdata.h.
8.13.3.14 x
double* x
state (dimension: nt x nx, column-major)
Definition at line 73 of file rdata.h.
8.13.3.15 sx
double* sx
parameter derivative of state (dimension: nt x nx x nplist, column-major)
Definition at line 76 of file rdata.h.
```

```
8.13.3.16 y
double* y
observable (dimension: nt x ny, column-major)
Definition at line 79 of file rdata.h.
8.13.3.17 sigmay
double* sigmay
observable standard deviation (dimension: nt x ny, column-major)
Definition at line 82 of file rdata.h.
8.13.3.18 sy
double* sy
parameter derivative of observable (dimension: nt x ny x nplist, column-major)
Definition at line 85 of file rdata.h.
8.13.3.19 ssigmay
double* ssigmay
parameter derivative of observable standard deviation (dimension: nt x ny x nplist, column-major)
Definition at line 88 of file rdata.h.
8.13.3.20 numsteps
double* numsteps
number of integration steps forward problem (dimension: nt)
Definition at line 91 of file rdata.h.
```

8.13.3.21 numstepsB double* numstepsB number of integration steps backward problem (dimension: nt) Definition at line 94 of file rdata.h. 8.13.3.22 numrhsevals double* numrhsevals number of right hand side evaluations forward problem (dimension: nt) Definition at line 97 of file rdata.h. 8.13.3.23 numrhsevalsB double* numrhsevalsB number of right hand side evaluations backwad problem (dimension: nt) Definition at line 100 of file rdata.h. 8.13.3.24 numerrtestfails double* numerrtestfails number of error test failures forward problem (dimension: nt) Definition at line 103 of file rdata.h. 8.13.3.25 numerrtestfailsB double* numerrtestfailsB number of error test failures backwad problem (dimension: nt) Definition at line 106 of file rdata.h.

8.13.3.26 numnonlinsolvconvfails double* numnonlinsolvconvfails number of linear solver convergence failures forward problem (dimension: nt) Definition at line 109 of file rdata.h. 8.13.3.27 numnonlinsolvconvfailsB double* numnonlinsolvconvfailsB number of linear solver convergence failures backwad problem (dimension: nt) Definition at line 112 of file rdata.h. 8.13.3.28 order double* order employed order forward problem (dimension: nt) Definition at line 115 of file rdata.h. 8.13.3.29 newton status double* newton_status flag indicating success of Newton solver Definition at line 118 of file rdata.h. 8.13.3.30 newton_numsteps double* newton_numsteps number of Newton steps for steady state problem

Definition at line 124 of file rdata.h.

```
8.13.3.31 newton_numlinsteps
double* newton_numlinsteps
number of linear steps by Newton step for steady state problem
Definition at line 127 of file rdata.h.
8.13.3.32 xss
double* xss
steady state found be Newton solver
Definition at line 130 of file rdata.h.
8.13.3.33 IIh
double* 11h
likelihood value (double[1])
Definition at line 133 of file rdata.h.
8.13.3.34 chi2
double* chi2
chi2 value (double[1])
Definition at line 136 of file rdata.h.
8.13.3.35 sllh
double* sllh
parameter derivative of likelihood (dimension: nplist)
Definition at line 139 of file rdata.h.
```

```
8.13.3.36 s2llh
double* s211h
second order parameter derivative of likelihood (dimension: (nJ-1) x nplist, column-major)
Definition at line 142 of file rdata.h.
8.13.3.37 status
double* status
status code (double[1])
Definition at line 145 of file rdata.h.
8.13.3.38 np
const int np
total number of model parameters
Definition at line 189 of file rdata.h.
8.13.3.39 nk
const int nk
number of fixed parameters
Definition at line 191 of file rdata.h.
8.13.3.40 nx
const int nx
number of states
Definition at line 193 of file rdata.h.
```

```
8.13.3.41 nxtrue
const int nxtrue
number of states in the unaugmented system
Definition at line 195 of file rdata.h.
8.13.3.42 ny
const int ny
number of observables
Definition at line 197 of file rdata.h.
8.13.3.43 nytrue
const int nytrue
number of observables in the unaugmented system
Definition at line 199 of file rdata.h.
8.13.3.44 nz
const int nz
number of event outputs
Definition at line 201 of file rdata.h.
8.13.3.45 nztrue
const int nztrue
number of event outputs in the unaugmented system
Definition at line 203 of file rdata.h.
```

```
8.13.3.46 ne
const int ne
number of events
Definition at line 205 of file rdata.h.
8.13.3.47 nJ
const int nJ
dimension of the augmented objective function for 2nd order ASA
Definition at line 207 of file rdata.h.
8.13.3.48 nplist
const int nplist
number of parameter for which sensitivities were requested
Definition at line 210 of file rdata.h.
8.13.3.49 nmaxevent
const int nmaxevent
maximal number of occuring events (for every event type)
Definition at line 212 of file rdata.h.
8.13.3.50 nt
const int nt
number of considered timepoints
Definition at line 214 of file rdata.h.
```

```
8.13.3.51 newton_maxsteps
const int newton_maxsteps
maximal number of newton iterations for steady state calculation
Definition at line 216 of file rdata.h.
8.13.3.52 pscale
const AMICI_parameter_scaling pscale
scaling of parameterization (lin,log,log10)
Definition at line 218 of file rdata.h.
8.13.3.53 o2mode
const AMICI_o2mode o2mode
flag indicating whether second order sensitivities were requested
Definition at line 220 of file rdata.h.
8.13.3.54 sensi
const AMICI_sensi_order sensi
sensitivity order
Definition at line 222 of file rdata.h.
8.13.3.55 sensi_meth
const AMICI_sensi_meth sensi_meth
sensitivity method
```

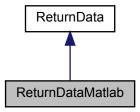
Definition at line 224 of file rdata.h.

8.14 ReturnDataMatlab Class Reference

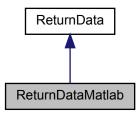
The ReturnDataMatlab class sets up ReturnData to be returned by the MATLAB mex functions. Memory is allocated using matlab functions.

```
#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

8.14.1 Detailed Description

Definition at line 14 of file returndata_matlab.h.

8.14.2 Member Function Documentation

8.14.2.1 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 32 of file returndata_matlab.cpp.

8.14.2.2 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 43 of file returndata_matlab.cpp.

8.14.2.3 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

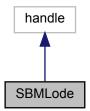
Reimplemented from ReturnData.

Definition at line 55 of file returndata_matlab.cpp.

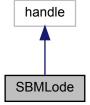
8.15 SBMLode Class Reference

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

Inheritance diagram for SBMLode:



Collaboration diagram for SBMLode:



Public Member Functions

• SBMLode (matlabtypesubstitute filename)

SBMLode extracts information from an SBML definition and stores it in a symbolic format.

noret::substitute checkODE (matlabtypesubstitute filename, matlabtypesubstitute this)

checkODE checks whether the length of various variable names exceeds namelengthmax (would cause troube with symbolic processing later on).

• noret::substitute writeAMICI (matlabtypesubstitute modelname)

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

Public Attributes

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

states

matlabtypesubstitute observable = sym.empty("")

observables

• matlabtypesubstitute observable_name = sym.empty("")

names of observables

matlabtypesubstitute param = sym.empty("")

parameter names

matlabtypesubstitute parameter = sym.empty("")

parameter expressions

matlabtypesubstitute constant = sym.empty("")

constants

• matlabtypesubstitute reaction = sym.empty("")

reactions

matlabtypesubstitute compartment = sym.empty("")

compartments

• matlabtypesubstitute volume = sym.empty("")

compartment volumes

matlabtypesubstitute kvolume = sym.empty("")

condition volumes

• matlabtypesubstitute initState = sym.empty("")

initial condition of states

• matlabtypesubstitute condition = sym.empty("")

condition

matlabtypesubstitute flux = sym.empty("")

reaction fluxes

matlabtypesubstitute stochiometry = sym.empty("")

reaction stochiometry

matlabtypesubstitute xdot = sym.empty("")

right hand side of reconstructed differential equation

matlabtypesubstitute trigger = sym.empty("")

event triggers

matlabtypesubstitute bolus = sym.empty("")

event boli

matlabtypesubstitute funmath = cell.empty("")

mathematical experessions for function

- matlabtypesubstitute **funarg** = cell.empty("")
- matlabtypesubstitute time_symbol = char.empty("")

symbol of time

• matlabtypesubstitute pnom = double.empty("")

nominal parameters

matlabtypesubstitute knom = double.empty("")

nominal conditions

8.15.1 Detailed Description

Definition at line 17 of file SBMLode.m.

8.15.2 Constructor & Destructor Documentation

8.15.2.1 SBMLode()

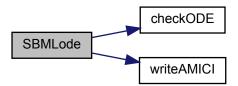
```
SBMLode ( {\tt matlabtypesubstitute}\ filename\ )
```

Parameters

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

Definition at line 201 of file SBMLode.m.

Here is the call graph for this function:



8.15.3 Member Function Documentation

8.15.3.1 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:



8.15.4 Member Data Documentation

```
8.15.4.1 state
```

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

Default: sym.empty("")

Definition at line 28 of file SBMLode.m.

8.15.4.2 observable

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

Default: sym.empty("")

Definition at line 36 of file SBMLode.m.

8.15.4.3 observable_name

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

Default: sym.empty("")

Definition at line 44 of file SBMLode.m.

```
8.15.4.4 param
param = sym.empty("")
Default: sym.empty("")
Definition at line 52 of file SBMLode.m.
8.15.4.5 parameter
parameter = sym.empty("")
Default: sym.empty("")
Definition at line 60 of file SBMLode.m.
8.15.4.6 constant
constant = sym.empty("")
Default: sym.empty("")
Definition at line 68 of file SBMLode.m.
8.15.4.7 reaction
reaction = sym.empty("")
Default: sym.empty("")
Definition at line 76 of file SBMLode.m.
8.15.4.8 compartment
```

Definition at line 84 of file SBMLode.m.

compartment = sym.empty("")

Default: sym.empty("")

```
8.15.4.9 volume
volume = sym.empty("")
Default: sym.empty("")
Definition at line 92 of file SBMLode.m.
8.15.4.10 kvolume
kvolume = sym.empty("")
Default: sym.empty("")
Definition at line 100 of file SBMLode.m.
8.15.4.11 initState
initState = sym.empty("")
Default: sym.empty("")
Definition at line 108 of file SBMLode.m.
8.15.4.12 condition
condition = sym.empty("")
Default: sym.empty("")
Definition at line 116 of file SBMLode.m.
8.15.4.13 flux
flux = sym.empty("")
```

Definition at line 124 of file SBMLode.m.

Default: sym.empty("")

```
8.15.4.14 stochiometry
stochiometry = sym.empty("")
Default: sym.empty("")
Definition at line 132 of file SBMLode.m.
8.15.4.15 xdot
xdot = sym.empty("")
Default: sym.empty("")
Definition at line 140 of file SBMLode.m.
8.15.4.16 trigger
trigger = sym.empty("")
Default: sym.empty("")
Definition at line 148 of file SBMLode.m.
8.15.4.17 bolus
bolus = sym.empty("")
Default: sym.empty("")
Definition at line 156 of file SBMLode.m.
8.15.4.18 funmath
```

0.13.4.10 IUIIIIIaiii

funmath = cell.empty("")

Default: cell.empty("")

Definition at line 164 of file SBMLode.m.

8.15.4.19 time_symbol

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

Default: char.empty("")

Definition at line 174 of file SBMLode.m.

8.15.4.20 pnom

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

Default: double.empty("")

Definition at line 182 of file SBMLode.m.

8.15.4.21 knom

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

Default: double.empty("")

Definition at line 190 of file SBMLode.m.

8.16 Solver Class Reference

Solver class.

```
#include <amici_solver.h>
```

Public Member Functions

- int setupAMI (UserData *udata, TempData *tdata, Model *model)
 setupAMIs initialises the ami memory object
- int setupAMIB (UserData *udata, TempData *tdata, Model *model)
- virtual int AMIGetSens (realtype *tret, N_Vector *yySout)=0
- int getDiagnosis (int it, ReturnData *rdata)
- int getDiagnosisB (int it, ReturnData *rdata, TempData *tdata)
- virtual int AMIGetRootInfo (int *rootsfound)=0
- virtual int AMIReInit (realtype t0, N Vector yy0, N Vector yp0)=0
- virtual int AMISensReInit (int ism, N_Vector *yS0, N_Vector *ypS0)=0
- virtual int AMICalcIC (realtype tout1)=0
- virtual int AMICalcICB (int which, realtype tout1, N_Vector xB, N_Vector dxB)=0
- virtual int **AMISolve** (realtype tout, N_Vector yret, N_Vector ypret, realtype *tret, int itask)=0
- virtual int AMISolveF (realtype tout, N_Vector yret, N_Vector ypret, realtype *tret, int itask, int *ncheckPtr)=0
- virtual int AMISolveB (realtype tBout, int itaskB)=0
- virtual int AMISetStopTime (realtype tstop)=0
- virtual int **AMIRootInit** (int nrtfn, RootFn ptr)=0
- virtual int AMIReInitB (int which, realtype tB0, N_Vector yyB0, N_Vector ypB0)=0
- virtual int AMIGetB (int which, realtype *tret, N Vector yy, N Vector yp)=0
- virtual int AMIGetQuadB (int which, realtype *tret, N_Vector qB)=0
- virtual int AMIQuadReInitB (int which, N_Vector yQB0)=0

Static Public Member Functions

- static int **fqBdot** (realtype t, N_Vector x, N_Vector xB, N_Vector qBdot, void *user_data)
- static 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)
- static int **fJSparse** (realtype t, N_Vector x, N_Vector xdot, SIsMat J, void *user_data, N_Vector tmp1, N_Vector tmp2, N_Vector tmp3)
- static int fJBand (long N, long mupper, long mlower, realtype t, N_Vector x, N_Vector xdot, DlsMat J, void *user_data, N_Vector tmp1, N_Vector tmp2, N_Vector tmp3)
- static int fJv (N_Vector v, N_Vector Jv, realtype t, N_Vector x, N_Vector xdot, void *user_data, N_Vector tmp)
- static int **fJB** (long 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)
- static 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)
- static int fJBandB (long NeqBdot, long mupper, long 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)
- static 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)

Protected Member Functions

- virtual int wrap_init (N_Vector x, N_Vector dx, realtype t)=0
- virtual int wrap_binit (int which, N Vector xB, N Vector dxB, realtype t)=0
- virtual int wrap_qbinit (int which, N_Vector qBdot)=0
- virtual int wrap RootInit (int ne)=0
- virtual int wrap_SensInit1 (N_Vector *sx, N_Vector *sdx, UserData *udata)=0
- virtual int wrap_SetDenseJacFn ()=0
- virtual int wrap_SetSparseJacFn ()=0
- virtual int wrap_SetBandJacFn ()=0
- virtual int wrap SetJacTimesVecFn ()=0
- virtual int wrap SetDenseJacFnB (int which)=0
- virtual int wrap SetSparseJacFnB (int which)=0
- virtual int wrap_SetBandJacFnB (int which)=0
- virtual int wrap_SetJacTimesVecFnB (int which)=0
- virtual void * AMICreate (int lmm, int iter)=0
- virtual int AMISStolerances (double rtol, double atol)=0
- virtual int AMISensEEtolerances ()=0
- virtual int AMISetSensErrCon (bool error corr)=0
- virtual int AMISetQuadErrConB (int which, bool flag)=0
- virtual int AMISetErrHandlerFn ()=0
- virtual int AMISetUserData (void *user data)=0
- virtual int AMISetUserDataB (int which, void *user data)=0
- virtual int AMISetMaxNumSteps (long int mxsteps)=0
- virtual int AMISetStabLimDet (int stldet)=0
- virtual int AMISetStabLimDetB (int which, int stldet)=0
- virtual int AMISetId (Model *model)=0
- virtual int AMISetSuppressAlg (bool flag)=0
- virtual int AMISetSensParams (realtype *p, realtype *pbar, int *plist)=0
- virtual int AMIGetDky (realtype t, int k, N_Vector dky)=0
- virtual void AMIFree (void **mem)
- virtual int AMIAdjInit (long int steps, int interp)=0
- virtual int AMICreateB (int Imm, int iter, int *which)=0
- virtual int AMISStolerancesB (int which, realtype relTolB, realtype absTolB)=0
- virtual int AMIQuadSStolerancesB (int which, realtype reltoIQB, realtype abstoIQB)=0

- virtual int AMISetMaxNumStepsB (int which, long int mxstepsB)=0
- virtual int AMIDense (int nx)=0
- virtual int AMIDenseB (int which, int nx)=0
- virtual int AMIBand (int nx, int ubw, int lbw)=0
- virtual int AMIBandB (int which, int nx, int ubw, int lbw)=0
- virtual int AMIDiag ()=0
- virtual int AMIDiagB (int which)=0
- virtual int AMISpgmr (int prectype, int maxl)=0
- virtual int AMISpgmrB (int which, int prectype, int maxl)=0
- virtual int AMISpbcg (int prectype, int maxl)=0
- virtual int AMISpbcgB (int which, int prectype, int maxl)=0
- virtual int AMISptfqmr (int prectype, int maxl)=0
- virtual int AMISptfqmrB (int which, int prectype, int maxl)=0
- virtual int AMIKLU (int nx, int nnz, int sparsetype)=0
- virtual int AMIKLUSetOrdering (int ordering)=0
- virtual int AMIKLUSetOrderingB (int which, int ordering)=0
- virtual int AMIKLUB (int which, int nx, int nnz, int sparsetype)=0
- virtual int AMIGetNumSteps (void *ami_mem, long int *numsteps)=0
- virtual int AMIGetNumRhsEvals (void *ami mem, long int *numrhsevals)=0
- virtual int AMIGetNumErrTestFails (void *ami_mem, long int *numerrtestfails)=0
- virtual int AMIGetNumNonlinSolvConvFails (void *ami mem, long int *numnonlinsolvconvfails)=0
- virtual int AMIGetLastOrder (void *ami_mem, int *order)=0
- virtual void * AMIGetAdjBmem (void *ami_mem, int which)=0
- int setLinearSolver (const UserData *udata, Model *model)

Static Protected Member Functions

 static void wrap_ErrHandlerFn (int error_code, const char *module, const char *function, char *msg, void *eh_data)

Protected Attributes

```
• void * ami_mem = nullptr
```

8.16.1 Detailed Description

provides a generic interface to CVode and IDA solvers, individual realizations are realized in the CVodeSolver and the IDASolver class.

Definition at line 20 of file amici_solver.h.

8.16.2 Member Function Documentation

8.16.2.1 setupAMI()

Parameters

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

Returns

ami_mem pointer to the cvodes/idas memory block

Definition at line 13 of file amici_solver.cpp.

Here is the caller graph for this function:



8.16.2.2 setupAMIB()

setupAMIB initialises the AMI memory object for the backwards problem

Parameters

out	status	flag indicating success of execution Type : int
in	ami_mem	pointer to the solver memory object of the forward problem
in	udata	pointer to the user data struct Type : UserData
in	tdata	pointer to the temporary data struct Type : TempData

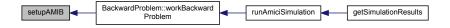
Returns

status flag indicating success of execution

Type: int

Definition at line 113 of file amici_solver.cpp.

Here is the caller graph for this function:



8.16.2.3 getDiagnosis()

getDiagnosis extracts diagnosis information from solver memory block and writes them into the return data struct

Parameters



Definition at line 322 of file amici_solver.cpp.

Here is the caller graph for this function:



8.16.2.4 getDiagnosisB()

getDiagnosisB extracts diagnosis information from solver memory block and writes them into the return data struct for the backward problem

Parameters

in	it	time-point index Type : int
in	ami_mem	pointer to the solver memory block
		Type: *void

Parameters

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

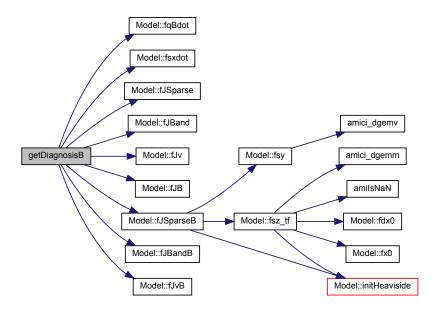
Returns

status flag indicating success of execution

Type: int

Definition at line 352 of file amici_solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.16.3 Member Data Documentation

8.16.3.1 ami_mem

```
void* ami_mem = nullptr [protected]
```

pointer to ami memory block

Definition at line 255 of file amici_solver.h.

8.17 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)
- static int getNewtonStep (UserData *udata, ReturnData *rdata, TempData *tdata, int ntry, int nnewt, N_Vector ns_delta, Model *model)
- 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)

8.17.1 Detailed Description

Definition at line 19 of file steadystateproblem.h.

8.17.2 Member Function Documentation

8.17.2.1 workSteadyStateProblem()

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

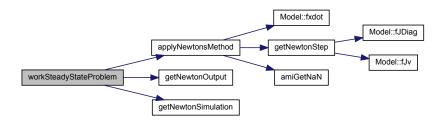
tries to determine the steady state of the ODE system by a Newton solver uses forward intergration, if the Newton solver fails

Parameters

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

Definition at line 18 of file steadystateproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.17.2.2 applyNewtonsMethod()

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

Parameters

in	udata	pointer to the user data struct
		Type: UserData

Parameters

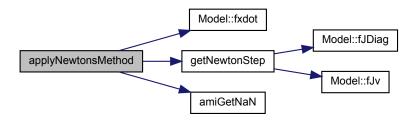
in	tdata	pointer to the temporary data struct
		Type: TempData
out	tdata	pointer to the temporary data struct
		Type: TempData
out	rdata	pointer to the return data struct
		Type: ReturnData
in	newton_try	integer for the try number of the Newton solver

Returns

void

Definition at line 71 of file steadystateproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.17.2.3 getNewtonStep()

getNewtonStep acomputes the Newton Step by solving a 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
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

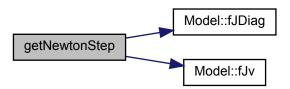
Returns

int status flag indicating success of execution

Type: int

Definition at line 209 of file steadystateproblem.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



8.17.2.4 getNewtonOutput()

getNewtonOutput stores the output of the Newton solver run.

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	newton_status	integer flag indicating the run of the Newton solver
in	run_time	double computation time of the Newton solver

Returns

int status flag indicating success of execution

Type: int

Definition at line 348 of file steadystateproblem.cpp.

Here is the caller graph for this function:



8.17.2.5 getNewtonSimulation()

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

getNewtonSimulation solves the forward problem, if the first Newton solver run did not succeed.

Parameters

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

Returns

int status flag indicating success of execution

Type: int

Definition at line 384 of file steadystateproblem.cpp.

Here is the caller graph for this function:

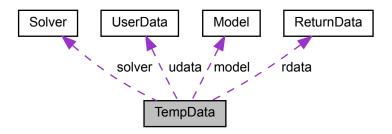


8.18 TempData Class Reference

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
- realtype * dJzdsigma
- realtype * dJrzdz
- realtype * dJrzdsigma
- realtype * dzdx
- realtype * dzdp
- realtype * drzdx
- realtype * drzdp
- realtype * dydp
- realtype * dydx
- realtype * yS0
- realtype * sigmay
- realtype * dsigmaydp
- realtype * sigmaz
- realtype * dsigmazdp
- int * rootsfound
- int * rootidx
- int * nroots
- realtype * rootvals
- realtype * h
- realtype * h_udata
- realtype * deltax
- realtype * deltasx
- realtype * deltaxB
- realtype * deltaqB
- · int which
- realtype * discs
- realtype * irdiscs
- 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
8.18.1 Detailed Description
Definition at line 17 of file tdata.h.
8.18.2 Member Data Documentation
8.18.2.1 p
```

realtype* p = nullptr

parameter array, unscaled

Definition at line 28 of file tdata.h.

```
8.18.2.2 t
realtype t
```

current time

Definition at line 31 of file tdata.h.

```
8.18.2.3 x
```

N_Vector x

state vector

Definition at line 34 of file tdata.h.

```
8.18.2.4 x_old
N_Vector x_old
old state vector
Definition at line 36 of file tdata.h.
8.18.2.5 x_disc
N_Vector* x_disc
array of state vectors at discontinuities
Definition at line 38 of file tdata.h.
8.18.2.6 xdot_disc
N_Vector* xdot_disc
array of differential state vectors at discontinuities
Definition at line 40 of file tdata.h.
8.18.2.7 xdot_old_disc
N_Vector* xdot_old_disc
array of old differential state vectors at discontinuities
Definition at line 42 of file tdata.h.
8.18.2.8 dx
N_Vector dx
differential state vector
Definition at line 44 of file tdata.h.
```

8.18.2.9 dx_old
N_Vector dx_old
old differential state vector
Definition at line 46 of file tdata.h.
8.18.2.10 xdot
N_Vector xdot
time derivative state vector
Definition at line 48 of file tdata.h.
8.18.2.11 xdot_old
N_Vector xdot_old
old time derivative state vector
Definition at line 50 of file tdata.h.
8.18.2.12 xB
N_Vector xB
adjoint state vector
Definition at line 52 of file tdata.h.
8.18.2.13 xB_old
N_Vector xB_old
old adjoint state vector
Definition at line 54 of file tdata.h.

8.18.2.14 dxB
N_Vector dxB
differential adjoint state vector
Definition at line 56 of file tdata.h.
3.18.2.15 xQB
N_Vector xQB
quadrature state vector
Definition at line 58 of file tdata.h.
3.18.2.16 xQB_old
N_Vector xQB_old
old quadrature state vector
Definition at line 60 of file tdata.h.
8.18.2.17 sx
N_Vector* sx
sensitivity state vector array
Definition at line 62 of file tdata.h.
B.18.2.18 sdx
N_Vector* sdx
differential sensitivity state vector array
Definition at line 64 of file tdata.h.

```
8.18.2.19 Jtmp
DlsMat Jtmp
Jacobian
Definition at line 66 of file tdata.h.
8.18.2.20 IIhS0
realtype* llhS0
parameter derivative of likelihood array
Definition at line 69 of file tdata.h.
8.18.2.21 Jy
realtype* Jy
data likelihood
Definition at line 71 of file tdata.h.
8.18.2.22 dJydp
realtype* dJydp
parameter derivative of data likelihood
Definition at line 73 of file tdata.h.
8.18.2.23 dJydy
realtype* dJydy
observable derivative of data likelihood
Definition at line 75 of file tdata.h.
```

8.18.2.24 dJydsigma realtype* dJydsigma observable sigma derivative of data likelihood Definition at line 77 of file tdata.h. 8.18.2.25 dJydx realtype* dJydx state derivative of data likelihood Definition at line 79 of file tdata.h. 8.18.2.26 Jz realtype* Jz event likelihood Definition at line 81 of file tdata.h. 8.18.2.27 dJzdp realtype* dJzdp parameter derivative of event likelihood Definition at line 83 of file tdata.h. 8.18.2.28 dJzdx realtype* dJzdx state derivative of event likelihood Definition at line 85 of file tdata.h.

```
8.18.2.29 dJzdz
realtype* dJzdz
event ouput derivative of event likelihood
Definition at line 87 of file tdata.h.
8.18.2.30 dJzdsigma
realtype* dJzdsigma
event sigma derivative of event likelihood
Definition at line 89 of file tdata.h.
8.18.2.31 dJrzdz
realtype* dJrzdz
event ouput derivative of event likelihood at final timepoint
Definition at line 91 of file tdata.h.
8.18.2.32 dJrzdsigma
realtype* dJrzdsigma
event sigma derivative of event likelihood at final timepoint
Definition at line 93 of file tdata.h.
8.18.2.33 dzdx
```

realtype* dzdx

state derivative of event output

Definition at line 95 of file tdata.h.

8.18.2.34 dzdp realtype* dzdp parameter derivative of event output Definition at line 97 of file tdata.h. 8.18.2.35 drzdx realtype* drzdx state derivative of event timepoint Definition at line 99 of file tdata.h. 8.18.2.36 drzdp realtype* drzdp parameter derivative of event timepoint Definition at line 101 of file tdata.h. 8.18.2.37 dydp realtype* dydp parameter derivative of observable Definition at line 103 of file tdata.h. 8.18.2.38 dydx realtype* dydx state derivative of observable Definition at line 105 of file tdata.h.

```
8.18.2.39 yS0
realtype* yS0
initial sensitivity of observable
Definition at line 107 of file tdata.h.
8.18.2.40 sigmay
realtype* sigmay
data standard deviation
Definition at line 109 of file tdata.h.
8.18.2.41 dsigmaydp
realtype* dsigmaydp
parameter derivative of data standard deviation
Definition at line 111 of file tdata.h.
8.18.2.42 sigmaz
realtype* sigmaz
event standard deviation
Definition at line 113 of file tdata.h.
8.18.2.43 dsigmazdp
realtype* dsigmazdp
parameter derivative of event standard deviation
```

Definition at line 115 of file tdata.h.

8.18.2.44 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 gi 0 if not.

Definition at line 121 of file tdata.h.

8.18.2.45 rootidx

```
int* rootidx
```

array of index which root has been found

Definition at line 123 of file tdata.h.

8.18.2.46 nroots

```
int* nroots
```

array of number of found roots for a certain event type

Definition at line 125 of file tdata.h.

8.18.2.47 rootvals

```
realtype* rootvals
```

array of values of the root function

Definition at line 127 of file tdata.h.

8.18.2.48 h

realtype* h

temporary rootval storage to check crossing in secondary event

Definition at line 129 of file tdata.h.

8.18.2.49 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 133 of file tdata.h. 8.18.2.50 deltax realtype* deltax change in x Definition at line 136 of file tdata.h. 8.18.2.51 deltasx realtype* deltasx change in sx Definition at line 138 of file tdata.h. 8.18.2.52 deltaxB realtype* deltaxB change in xB Definition at line 140 of file tdata.h. 8.18.2.53 deltaqB realtype* deltaqB

Definition at line 142 of file tdata.h.

change in qB

```
8.18.2.54 which
int which
integer for indexing of backwards problems
Definition at line 145 of file tdata.h.
8.18.2.55 discs
realtype* discs
array containing the time-points of discontinuities
Definition at line 148 of file tdata.h.
8.18.2.56 irdiscs
realtype* irdiscs
array containing the index of discontinuities
Definition at line 150 of file tdata.h.
8.18.2.57 J
SlsMat J = NULL
tempory storage of Jacobian data across functions
Definition at line 153 of file tdata.h.
8.18.2.58 dxdotdp
realtype* dxdotdp = NULL
tempory storage of dxdotdp data across functions
```

Definition at line 155 of file tdata.h.

```
8.18.2.59 w
```

```
realtype* w = NULL
```

tempory storage of w data across functions

Definition at line 157 of file tdata.h.

8.18.2.60 dwdx

```
realtype* dwdx = NULL
```

tempory storage of dwdx data across functions

Definition at line 159 of file tdata.h.

8.18.2.61 dwdp

```
realtype* dwdp = NULL
```

tempory storage of dwdp data across functions

Definition at line 161 of file tdata.h.

8.18.2.62 M

```
realtype* M = NULL
```

tempory storage of M data across functions

Definition at line 163 of file tdata.h.

8.18.2.63 dfdx

```
realtype* dfdx = NULL
```

tempory storage of dfdx data across functions

Definition at line 165 of file tdata.h.

```
8.18.2.64 stau
realtype* stau = NULL
tempory storage of stau data across functions
Definition at line 167 of file tdata.h.
8.18.2.65 nplist
int nplist
number of parameters, copied from udata, necessary for deallocation
Definition at line 170 of file tdata.h.
8.18.2.66 iroot
int iroot = 0
current root index, will be increased during the forward solve and decreased during backward solve
Definition at line 173 of file tdata.h.
8.18.2.67 nan_dxdotdp
booleantype nan_dxdotdp = false
flag indicating whether a NaN in dxdotdp has been reported
Definition at line 176 of file tdata.h.
8.18.2.68 nan_J
booleantype nan_J = false
```

flag indicating whether a NaN in J has been reported

Definition at line 178 of file tdata.h.

```
8.18.2.69 nan_JDiag
booleantype nan_JDiag = false
flag indicating whether a NaN in JDiag has been reported
Definition at line 180 of file tdata.h.
8.18.2.70 nan_JSparse
booleantype nan_JSparse = false
flag indicating whether a NaN in JSparse has been reported
Definition at line 182 of file tdata.h.
8.18.2.71 nan_xdot
booleantype nan_xdot = false
flag indicating whether a NaN in xdot has been reported
Definition at line 184 of file tdata.h.
8.18.2.72 nan xBdot
booleantype nan_xBdot = false
flag indicating whether a NaN in xBdot has been reported
Definition at line 186 of file tdata.h.
8.18.2.73 nan_qBdot
```

booleantype nan_qBdot = false

flag indicating whether a NaN in qBdot has been reported

Definition at line 188 of file tdata.h.

```
8.18.2.74 udata
const UserData* udata
attached UserData object
Definition at line 191 of file tdata.h.
8.18.2.75 model
Model* model
attached Model object
Definition at line 193 of file tdata.h.
8.18.2.76 rdata
ReturnData* rdata
attached ReturnData object
Definition at line 195 of file tdata.h.
8.18.2.77 solver
Solver* solver = nullptr
attached Solver object
Definition at line 197 of file tdata.h.
8.19 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 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 ()

8.19.1 Detailed Description

Definition at line 10 of file udata.h.

8.19.2 Member Function Documentation

8.19.2.1 print()

void print ()

function to print the contents of the UserData object

Definition at line 79 of file udata.cpp.

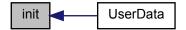
8.19.2.2 init()

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

function to initialize the UserData member variables

Definition at line 45 of file udata.cpp.

Here is the caller graph for this function:



8.19.3 Member Data Documentation

8.19.3.1 nmaxevent

int nmaxevent

maximal number of events to track

Definition at line 25 of file udata.h.

8.19.3.2 qpositivex

double* qpositivex

positivity flag

Definition at line 28 of file udata.h.

8.19.3.3 plist

int* plist

parameter selection and reordering

Definition at line 31 of file udata.h.

8.19.3.4 nplist
int nplist
number of parameters in plist
Definition at line 33 of file udata.h.
8.19.3.5 nt
int nt
number of timepoints
Definition at line 36 of file udata.h.
8.19.3.6 p
double* p
parameter array
Definition at line 39 of file udata.h.
8.19.3.7 k
double* k
constants array
Definition at line 42 of file udata.h.
8.19.3.8 pscale
AMICI_parameter_scaling pscale
parameter transformation of p
Definition at line 45 of file udata.h.

8.19.3.9 tstart
double tstart
starting time
Definition at line 48 of file udata.h.
8.19.3.10 ts
double* ts
timepoints
Definition at line 50 of file udata.h.
8.19.3.11 pbar
double* pbar
scaling of parameters
Definition at line 53 of file udata.h.
8.19.3.12 xbar
double* xbar
scaling of states
Definition at line 55 of file udata.h.
8.19.3.13 sensi
AMICI_sensi_order sensi
flag indicating whether sensitivities are supposed to be computed
Definition at line 58 of file udata.h.

8.19.3.14 atol double atol absolute tolerances for integration Definition at line 60 of file udata.h. 8.19.3.15 rtol double rtol relative tolerances for integration Definition at line 62 of file udata.h. 8.19.3.16 maxsteps int maxsteps maximum number of allowed integration steps Definition at line 64 of file udata.h. 8.19.3.17 newton_maxsteps int newton_maxsteps maximum number of allowed Newton steps for steady state computation Definition at line 66 of file udata.h. 8.19.3.18 newton_maxlinsteps int newton_maxlinsteps maximum number of allowed linear steps per Newton step for steady state computation Definition at line 68 of file udata.h.

8.19.3.19 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 74 of file udata.h.

8.19.3.20 sensi_meth

AMICI_sensi_meth sensi_meth

method for sensitivity computation

Definition at line 77 of file udata.h.

8.19.3.21 linsol

int linsol

linear solver specification

Definition at line 80 of file udata.h.

8.19.3.22 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 86 of file udata.h.

8.19.3.23 lmm

int 1mm

linear multistep method

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

Definition at line 92 of file udata.h.

9 File Documentation 187

8.19.3.24 iter int iter nonlinear solver specifies the type of nonlinear solver iteration and may be either CV NEWTON or CV FUNCTIONAL. Definition at line 98 of file udata.h. 8.19.3.25 stldet booleantype stldet flag controlling stability limit detection Definition at line 101 of file udata.h. 8.19.3.26 x0data double* x0data state initialisation Definition at line 104 of file udata.h. 8.19.3.27 sx0data double* sx0data sensitivity initialisation Definition at line 107 of file udata.h. 8.19.3.28 ordering int ordering state ordering Definition at line 110 of file udata.h.

9 File Documentation

9.1 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.

9.1.1 Function Documentation

9.1.1.1 amiwrap()

```
noret::substitute amiwrap ( {\tt matlabtypesubstitute}\ varargin\ )
```

Parameters

varargin

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

Required Parameters for varargin:

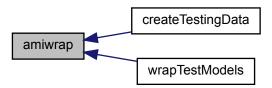
- modelname specifies the name of the model which will be later used for the naming of the simulation file
- symfun specifies a function which executes model definition see Model Definition for details
- tdir target directory where the simulation file should be placed **Default:** \$AMICIDIR/models/modelname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

Return values

<i>0≥liag</i> void	o2flag	void
----------------------	--------	------

Definition at line 17 of file amiwrap.m.

Here is the caller graph for this function:



9.2 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.

9.2.1 Function Documentation

9.2.1.1 SBML2AMICI()

Parameters

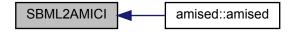
filename	name of the SBML file (withouth extension)]
modelname	name of the model, this will define the name of the output file (default: input filename)	Ī

Return values

modelname	void
modeliane	voiu

Definition at line 17 of file SBML2AMICI.m.

Here is the caller graph for this function:



9.3 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.

9.3.1 Function Documentation

9.3.1.1 computeBracketLevel()

Parameters

```
cstr input string
```

Return values

```
brl bracket levels
```

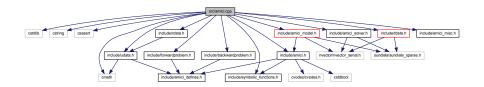
Definition at line 17 of file computeBracketLevel.m.

9.4 src/amici.cpp File Reference

core routines for integration

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

Include dependency graph for amici.cpp:



Macros

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

Functions

- int runAmiciSimulation (UserData *udata, const ExpData *edata, ReturnData *rdata, Model *model)
- void printErrMsgldAndTxt (const char *identifier, const char *msg,...)
- void printWarnMsgldAndTxt (const char *identifier, const char *msg,...)

Variables

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

9.4.1 Function Documentation

9.4.1.1 runAmiciSimulation()

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

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

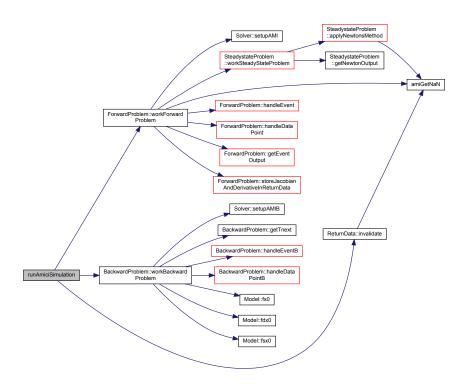
Returns

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:



9.4.1.2 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 73 of file amici.cpp.

9.4.1.3 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 84 of file amici.cpp.

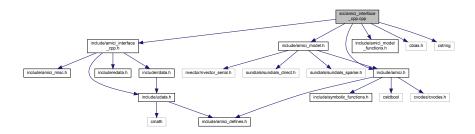
9.5 src/amici_interface_cpp.cpp File Reference

core routines for cpp interface

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

9.5.1 Function Documentation

9.5.1.1 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

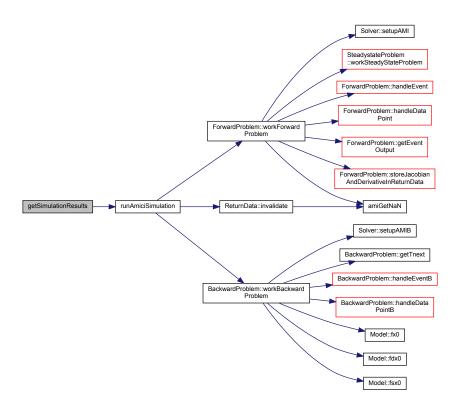
Returns

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:



9.5.1.2 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]

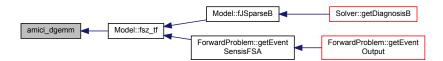
in	layout	can be AMICI_BLAS_ColMajor or AMICI_BLAS_RowMajor.
in	TransA	flag indicating whether A should be transposed before multiplication

Parameters

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)

Definition at line 63 of file amici_interface_cpp.cpp.

Here is the caller graph for this function:



9.5.1.3 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]

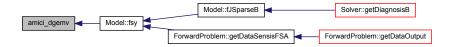
in	layout	can be AMICI_BLAS_ColMajor or AMICI_BLAS_RowMajor.
in	TransA	flag indicating whether A should be transposed before multiplication

Parameters

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

Definition at line 86 of file amici_interface_cpp.cpp.

Here is the caller graph for this function:

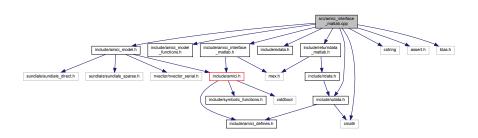


9.6 src/amici_interface_matlab.cpp File Reference

core routines for mex interface

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

Include dependency graph for amici_interface_matlab.cpp:



Macros

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

Functions

- void mexFunction (int nlhs, mxArray *plhs[], int nrhs, const mxArray *prhs[])
- UserData * userDataFromMatlabCall (const mxArray *prhs[], int nrhs, Model *model)
 userDataFromMatlabCall extracts information from the matlab call and returns the corresponding UserData struct
- char amici_blasCBlasTransToBlasTrans (AMICI_BLAS_TRANSPOSE trans)
- void amici_dgemm (AMICI_BLAS_LAYOUT layout, AMICI_BLAS_TRANSPOSE TransA, AMICI_BLAS_TRANSPOSE
 TransB, const int M, const int N, const int K, const double alpha, const double *A, const int lda, const double
 *B, const int ldb, const double beta, double *C, const int ldc)
- void amici_dgemv (AMICI_BLAS_LAYOUT layout, AMICI_BLAS_TRANSPOSE TransA, const int M, const int N, const double alpha, const double *A, const int lda, const double *X, const int incX, const double beta, double *Y, const int incY)
- ExpData * expDataFromMatlabCall (const mxArray *prhs[], const UserData *udata, Model *model)

9.6.1 Detailed Description

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

9.6.2 Macro Definition Documentation

9.6.2.1 readOptionScalar

Value:

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

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

Definition at line 30 of file amici_interface_matlab.cpp.

9.6.2.2 readOptionData

Value:

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

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

Definition at line 42 of file amici_interface_matlab.cpp.

9.6.3 Function Documentation

9.6.3.1 mexFunction()

```
void mexFunction (
    int nlhs,
    mxArray * plhs[],
    int nrhs,
    const mxArray * prhs[] )
```

mexFunction is the main interface function for the MATLAB interface. It reads in input data (udata and edata) and creates output data compound (rdata) and then calls the AMICI simulation routine to carry out numerical integration.

Parameters

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

Returns

void

Definition at line 65 of file amici_interface_matlab.cpp.

9.6.3.2 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 108 of file amici_interface_matlab.cpp.

9.6.3.3 amici_blasCBlasTransToBlasTrans()

amici_blasCBlasTransToBlasTrans translates AMICI_BLAS_TRANSPOSE values to CBlas readable strings

Parameters

in	trans	flag indicating transposition and complex conjugation
		Type: AMICI_BLAS_TRANSPOSE

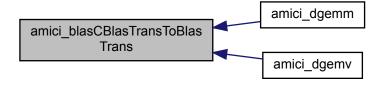
Returns

cblastrans CBlas readable CHAR indicating transposition and complex conjugation

Type: char

Definition at line 276 of file amici_interface_matlab.cpp.

Here is the caller graph for this function:



9.6.3.4 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]

in	layout	ut 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	in M number of rows in A/C		
in N number of columns in B/C		number of columns in B/C	
in K number of rows in B, number of columns in A		number of rows in B, number of columns in A	
in	alpha coefficient alpha		
in	Α	matrix A	
in Ida Ieading dimension of A (m or k)		leading dimension of A (m or k)	
in B matrix B		matrix B	
in Idb leading dimension of B (k or n)		leading dimension of B (k or n)	
in	beta	coefficient beta	
in,out	С	matrix C	
in	Idc leading dimension of C (m or n)		

Returns

void

Definition at line 308 of file amici_interface_matlab.cpp.

Here is the call graph for this function:



9.6.3.5 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]

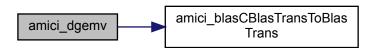
in	layout	always needs to be AMICI_BLAS_ColMajor.
in	TransA	flag indicating whether A should be transposed before multiplication
in	М	number of rows in A
in N number of columns in A		number of columns in A
in alpha coefficient alpha		coefficient alpha
in	Α	matrix A
in Ida leading dimension of A (m or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

Returns

void

Definition at line 347 of file amici_interface_matlab.cpp.

Here is the call graph for this function:



9.6.3.6 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 374 of file amici_interface_matlab.cpp.

9.7 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[])

9.7.1 Detailed Description

Author

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

9.7.2 Function Documentation

9.7.2.1 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.

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	in end2 0: default condition 1: specify the slopes at x	
in	in slope 1 slope at x[0]	
in	n slope2 slope at x[n-1]	
in	x[] the abscissas of the knots in strictly increasing of	
in	y[] the ordinates of the knots	
out	t b[] array of spline coefficients	
out	c[]	array of spline coefficients
out	d[]	array of spline coefficients

Return values

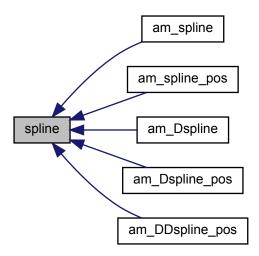
0	normal return	
1	less than two data points; cannot interpolate	
2	x[] are not in ascending order	

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 required 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 66 of file spline.cpp.

Here is the caller graph for this function:



9.7.2.2 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	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

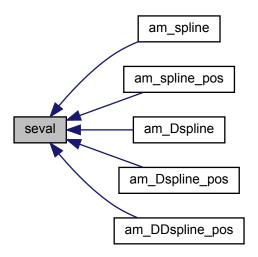
the value of the spline function at u

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 208 of file spline.cpp.

Here is the caller graph for this function:



9.7.2.3 sinteg()

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

Integrate the cubic spline function

```
S(xx) = y[i] + b[i] * w + c[i] * w * *2 + d[i] * w * *3 \text{ where } w = u - x[i] \text{ 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.

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.

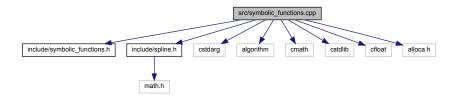
Definition at line 270 of file spline.cpp.

9.8 src/symbolic_functions.cpp File Reference

definition of symbolic functions

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

9.8.1 Detailed Description

This file contains definitions of various symbolic functions which

9.8.2 Function Documentation

9.8.2.1 amilsNaN()

c++ interface to the isNaN function

Parameters

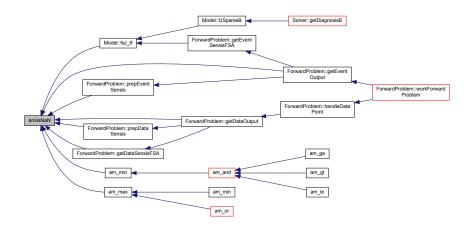
what argument

Returns

isnan(what)

Definition at line 33 of file symbolic_functions.cpp.

Here is the caller graph for this function:



9.8.2.2 amilsInf()

c++ interface to the isinf function

Parameters

<i>what</i> argument

Returns

isnan(what)

Definition at line 44 of file symbolic_functions.cpp.

9.8.2.3 amiGetNaN()

```
double amiGetNaN ( )
```

function returning nan

Returns

NaN

Definition at line 54 of file symbolic_functions.cpp.

Here is the caller graph for this function:



9.8.2.4 amilog()

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

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

Parameters



Returns

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

Definition at line 65 of file symbolic_functions.cpp.

9.8.2.5 dirac()

```
double dirac ( \mbox{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:



9.8.2.6 heaviside()

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

c implementation of matlab function heaviside

Parameters

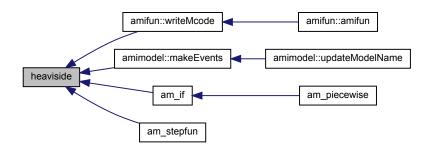
```
x argument
```

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:



9.8.2.7 sign()

```
double sign ( \mbox{double $x$}\ )
```

c implementation of matlab function sign

Parameters

```
x argument
```

Returns

0

Type: double

Definition at line 112 of file symbolic_functions.cpp.

9.8.2.8 am_min()

c implementation of matlab function min

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

Returns

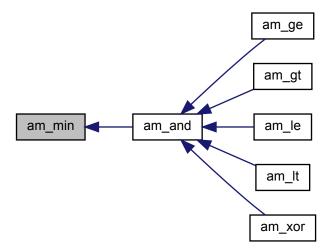
```
if(a < b) then a else b Type: double
```

Definition at line 133 of file symbolic_functions.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.8.2.9 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.

```
9.8.2.10 am_max()
```

```
double am_max ( \label{eq:double an_max} \mbox{double $a$,} \\ \mbox{double $c$ )}
```

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

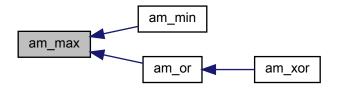
if(a > b) then a else b **Type**: double

Definition at line 179 of file symbolic_functions.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



9.8.2.11 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 200 of file symbolic_functions.cpp.

9.8.2.12 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

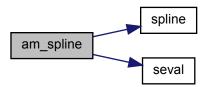
t	point at which the spline should be evaluate	
num	number of spline nodes	

Returns

spline(t)

Definition at line 228 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.8.2.13 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

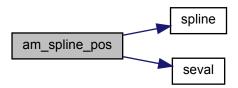
t point at which the spline should be evaluated	
num	number of spline nodes

Returns

spline(t)

Definition at line 279 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.8.2.14 am_Dspline()

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

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

Parameters

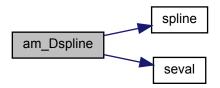
id	index of node to which the derivative of the corresponding spline coefficient should be computed
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

dsplinedp(t)

Definition at line 331 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.8.2.15 am_Dspline_pos()

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

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

Parameters

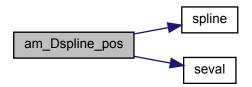
id	index of node to which the derivative of the corresponding spline coefficient should be computed	
t	point at which the spline should be evaluated	
num	number of spline nodes	

Returns

dsplinedp(t)

Definition at line 387 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.8.2.16 am_DDspline()

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

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

Parameters

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

Returns

ddspline(t)

Definition at line 452 of file symbolic_functions.cpp.

9.8.2.17 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

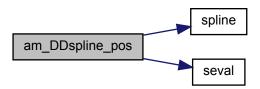
id1	index of node to which the first derivative of the corresponding spline coefficient should be computed
id2	index of node to which the second derivative of the corresponding spline coefficient should be computed
t	point at which the spline should be evaluated
num	number of spline nodes

Returns

ddspline(t)

Definition at line 469 of file symbolic_functions.cpp.

Here is the call graph for this function:



9.9 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

9.9.1 Function Documentation

9.9.1.1 am_and()

Parameters

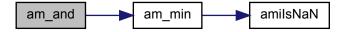
а	first input parameter
b	second input parameter

Return values

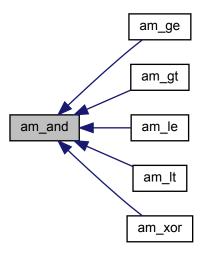
fun	logical value, negative for false, positive for true
-----	--

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:



9.10 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

9.10.1 Function Documentation

9.10.1.1 am_eq()

Parameters

varargin	elements for chain of equalities
----------	----------------------------------

Return values

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

Definition at line 17 of file am_eq.m.

9.11 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},...)

9.11.1 Function Documentation

9.11.1.1 am_ge()

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:



9.12 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},...)

9.12.1 Function Documentation

9.12.1.1 am_gt()

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

Parameters

varargin	chain of input parameters
_	

Return values

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

Definition at line 17 of file am_gt.m.

Here is the call graph for this function:



9.13 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

9.13.1 Function Documentation

9.13.1.1 am_if()

Parameters

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

Return values

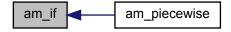
fun if condition	n is true truepart, else falsepart
------------------	------------------------------------

Definition at line 17 of file am_if.m.

Here is the call graph for this function:



Here is the caller graph for this function:



9.14 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},...)

9.14.1 Function Documentation

9.14.1.1 am_le()

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

Parameters

varargin	chain of input parameters
----------	---------------------------

Return values

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

Definition at line 17 of file am_le.m.

Here is the call graph for this function:



9.15 symbolic/am_lt.m File Reference

am_lt is the amici implementation of the n-ary mathml less than 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},...)

9.15.1 Function Documentation

9.15.1.1 am_lt()

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:



9.16 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

9.16.1 Function Documentation

9.16.1.1 am_max()

Parameters

а	first input parameter
b	second input parameter

Return values

fun maximum of a and b

Definition at line 17 of file am_max.m.

9.17 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

9.17.1 Function Documentation

9.17.1.1 am_min()

Parameters

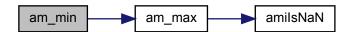
а	first input parameter
b	second input parameter

Return values

fun minimum of a and b	fun	minimum of a and b
--------------------------	-----	--------------------

Definition at line 17 of file am_min.m.

Here is the call graph for this function:



9.18 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

9.18.1 Function Documentation

9.18.1.1 am_or()

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

Parameters

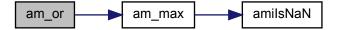
а	first input parameter
b	second input parameter

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:



9.19 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

9.19.1 Function Documentation

9.19.1.1 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:



9.20 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)

 $am_step \textit{fun} \ is \ the \ amici \ implementation \ of \ the \ step \ \textit{function}$

9.20.1 Function Documentation

9.20.1.1 am_stepfun()

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

Parameters

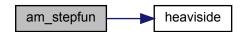
t	input variable
tstart	input variable value at which the step starts
vstart	value during the step
tend	input variable value at which the step end
vend	value after the step

Return values

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

Definition at line 17 of file am_stepfun.m.

Here is the call graph for this function:



9.21 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

9.21.1 Function Documentation

9.21.1.1 am_xor()

Parameters

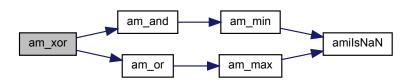
а	first input parameter
b	second input parameter

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:



9.22 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

9.23 tests/cpputest/wrapTestModels.m File Reference

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

Function	ns

noret::substitute wrapTestModels ()
 wrapTestModels calls amiwrap on all test models. currently necessary for continuous integrations to yield meaningful results

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