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, Iain S. Duff, *ACM Transactions on Mathematical Software*, Vol 30, Issue 3, 2004, pp 381 - 388. PDF

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

2 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.

2.1 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.

2.1.1 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()
```

2.1.2 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
.atol	absolute integration tolerance	1e-8
.rtol	relative integration tolerance	1e-8
.maxsteps	maximal number integration steps	1e4
.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.

2.1.3 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 ];
```

2.1.4 Parameters

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

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

Create the parameters vector

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

2.1.5 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];
```

2.1.6 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];
```

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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.

2.1.7 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];
```

2.1.8 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.

2.1.9 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

2.1.10 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.

2.1.11 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.y = p;
model.sym.x0 = x0;
model.sym.y = y;
model.sym.sigma_y = sigma_y;
model.sym.sigma_t = sigma_t;
```

2.2 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()

2.3 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.

2.3.1 Integration

Define a time vector:

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

Generate a parameter vector:

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

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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.

2.3.2 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.

2.3.3 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:

```
\begin{array}{lll} & \text{D.Y} = & [\text{NaN}(1,2)], \text{ones}(\text{length}(t)-1,2)]; \\ & \text{D.Sigma\_Y} = & [0.1*\text{ones}(\text{length}(t)-1,2), \text{NaN}(1,2)]; \\ & \text{D.T} = & \text{ones}(1,1); \\ & \text{D.Sigma\_T} = & \text{NaN}; \end{array}
```

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.

2.3.4 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:

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```
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.

3 Examples

In this section we include multiple examples on defining and simulating models.

Example 1: Forward Sensitivities for model with events and discontinuities.

Example 2: Forward Sensitivities for mRNA transfection model with bolus injection.

Example 3: Steady State Sensitivities.

Example 4: Adjoint Sensitivities for JAK/STAT model with parametric standard deviation.

Example 5: Adjoint Sensitivities for mRNA transfection model with bolus injection.

Example 6: Adjoint Sensitivities for simple model with analytic solution.

3.1 Example 1

3.1.1 Model Definition

```
function [model] = example_model_1_syms()
```

CVODES OPTIONS

```
% set the default absolute tolerance
model.atol = 1e-8;
% set the default relative tolerance
model.rtol = 1e-8;
% set the default maximum number of integration steps
model.maxsteps = 1e4;
% set the parametrisation of the problem options are 'log', 'log10' and
% 'lin' (default).
model.param = 'log10';
```

STATES

```
% create state syms
syms x1 x2 x3
% create state vector
x = [
x1 x2 x3
];
```

PARAMETERS (for these sensitivities will be computed)

```
% create parameter syms
syms p1 p2 p3 p4
% create parameter vector
p = [p1,p2,p3,p4];
```

CONSTANTS (for these no sensitivities will be computed) this part is optional and can be ommitted

```
% create parameter syms
syms k1 k2 k3 k4
% create parameter vector
k = [k1 k2 k3 k4];
```

SYSTEM EQUATIONS

```
% create symbolic variable for time
syms t

xdot = sym(zeros(size(x)));
% piecewise defined function
xdot(1) = -p1*heaviside(t-p4)*x1;
% inhomogeneous
xdot(2) = +p2*x1*exp(-0.1*t)-p3*x2;
xdot(3) = -1.5*x3;
```

INITIAL CONDITIONS

```
x0 = sym(zeros(size(x)));
x0(1) = k1;
x0(2) = k2;
x0(3) = k3;
```

OBSERVALES

```
y = sym(zeros(1,1));

y(1) = p4 * (x1+x2+x3);
```

EVENTS this part is optional and can be ommited

```
syms t
% events fire when there is a zero crossing of the root function
event(1) = amievent(x3-x2,0,t);
event(2) = amievent(x3-x1,0,t);
```

SYSTEM STRUCT

```
model.sym.x = x;
model.sym.k = k;
model.sym.xdot = xdot;
model.sym.p = p;
model.sym.y = x0;
model.sym.y = y;
model.event = event;

end

ans =
    atol: 1e-08
    rtol: 1e-08
    maxsteps: 10000
    param: 'log10'
    sym: [1x1 struct]
    event: [1x2 amievent]
```

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3.1.2 Simulation

```
clear
close all
clc
```

COMPILATION

```
[exdir,~,~]=fileparts(which('example_model_1.m'));
% compile the model
amiwrap('model_example_1','example_model_1_syms',exdir)
% add the model to the path
addpath(genpath([strrep(which('amiwrap.m'),'amiwrap.m','') 'models/model_example_1']))
Generating model struct ...
Parsing model struct ...
Error using amifun/getSyms
Too many output arguments.
Error in amimodel/getFun (line 42)
       [fun, this] = fun.getSyms(this);
Error in amimodel/checkDeps (line 38)
               this = this.getFun([],depsid);
this = this.getFun([],depsid);
Error in amimodel/getFun (line 25)
[this.cflag] = this.checkDeps(HTable,fun.deps);
Error in amimodel/parseModel (line 75)
       this = this.getFun(HTable, funsifun);
Error in amiwrap (line 70)
   model = model.parseModel();
Error in example_model_1 (line 9)
amiwrap('model_example_1','example_model_1_syms',exdir)
```

SIMULATION

```
% time vector
t = linspace(0,10,20);
p = [0.5;2;0.5;0.5];
k = [4,8,10,4];

options.sensi = 0;
options.cvode_maxsteps = le6;
options.nmaxevent = 2;
% load mex into memory
sol = simulate_model_example_1(t,log10(p),k,[],options);

tic
sol = simulate_model_example_1(t,log10(p),k,[],options);
disp(['Time elapsed with cvodes: ' num2str(toc) ])
```

ODF15S

```
figure
c_x = get(gca,'ColorOrder');
```

```
subplot (2,2,1)
for ix = 1:size(sol.x,2)
plot(t,sol.x(:,ix),'.-','Color',c_x(ix,:))
     hold on
    \verb"plot(t,X_odel5s(:,ix),'d','Color',c_x(ix,:))"
end
stem(sol.z(:,1),sol.z(:,1)*0+10,'r')
stem(sol.z(:,2),sol.z(:,2)*0+10,'k')
{\tt legend('x1','x1\_ode15s','x2','x2\_ode15s','x3','x3\_ode15s','x3=x2','x3=x1','Location','NorthEastOutside')}
legend boxoff
xlabel('time t')
ylabel('x')
box on
subplot (2,2,2)
plot(t,abs(sol.x-X_ode15s),'--')
set(gca,'YScale','log')
legend('error x1','error x2','error x3','Location','NorthEastOutside')
legend boxoff
ylabel('x')
subplot(2,2,3)
plot(t, sol.y,'.-','Color',c_x(1,:))
hold on
plot(t,p(4)*sum(X_ode15s,2),'d','Color',c_x(1,:))
legend('y1','y1_ode15s','Location','NorthEastOutside')
legend boxoff
xlabel('time t')
ylabel('y')
box on
subplot (2,2,4)
plot(t,sol.y-p(4) *sum(X_ode15s,2),'--')
set(gca,'YScale','log')
legend('error y1','Location','NorthEastOutside')
legend boxoff
xlabel('time t')
ylabel('y')
box on
set(gcf,'Position',[100 300 1200 500])
```

FORWARD SENSITIVITY ANALYSIS

```
options.sensi = 1;
sol = simulate_model_example_1(t,log10(p),k,[],options);
```

FINITE DIFFERENCES

```
eps = le-4;
xi = log10(p);
for ip = 1:4;
    xip = xi;
    xip(ip) = xip(ip) + eps;
    solp = simulate_model_example_1(t,xip,k,[],options);
    sx_fd(:,:,ip) = (solp.x - sol.x)/eps;
    sy_fd(:,:,ip) = (solp.y - sol.y)/eps;
    sz_fd(:,:,ip) = (solp.z - sol.z)/eps;
end
```

```
figure
for ip = 1:4
    subplot(4,2,ip*2-1)
    hold on
    for ix = 1:size(sol.x,2)
        plot(t,sol.sx(:,ix,ip),'.-','Color',c_x(ix,:))
        plot(t,sx_fd(:,ix,ip),'d','Color',c_x(ix,:))
    end
    legend('sx1','sx1_fd','sx2','sx2_fd','sx3','sx3_fd','Location','NorthEastOutside')
    legend boxoff
    title(['state sensitivity for p' num2str(ip)])
    xlabel('time t')
    ylabel('sx')
    box on
```

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```
subplot(4,2,ip*2)
           plot(t,abs(sol.sx(:,:,ip)-sx_fd(:,:,ip)),'--')
legend('error sx1','error sx2','error sx3','Location','NorthEastOutside')
           legend boxoff
           title(['state sensitivity for p' num2str(ip)])
           xlabel('time t')
           ylabel('error')
           set(gca,'YScale','log')
          box on
end
set(gcf,'Position',[100 300 1200 500])
figure
for ip = 1:4
           subplot (4,2,ip*2-1)
           hold on
           for iy = 1:size(sol.y, 2)
                     plot(t, sol.sy(:,iy,ip),'.-','Color',c_x(iy,:))
plot(t,sy_fd(:,iy,ip),'d','Color',c_x(iy,:))
           legend('syl','syl_fd','Location','NorthEastOutside')
           legend boxoff
           title(['observable sensitivity for p' num2str(ip)])
           xlabel('time t')
           ylabel('sy')
           box on
           subplot(4,2,ip*2)
           plot(t,abs(sol.sy(:,:,ip)-sy_fd(:,:,ip)),'--')
legend('error syl','Location','NorthEastOutside')
           legend boxoff
           title(['error observable sensitivity for p' num2str(ip)])
           xlabel('time t')
           ylabel('error')
           set(gca,'YScale','log')
           box on
end
set(gcf,'Position',[100 300 1200 500])
figure
for ip = 1:4
subplot(4,2,2*ip-1)
bar(1:options.nmaxevent,sol.sz(1:options.nmaxevent,:,ip).0.8)
hold on
\label{eq:bar(1:options.nmaxevent,:,ip),0.4)} $$ \log (x_3 = x_2', x_3 = x_1', x_3 = x_2', x_3 = x_1', 
legend boxoff
title(['event sensitivity for p' num2str(ip)])
xlabel('event #')
ylabel('sz')
box on
subplot(4,2,2*ip)
bar(1:options.nmaxevent,sol.sz(1:options.nmaxevent,:,ip)-sz_fd(1:options.nmaxevent,:,ip),0.8)
legend('error x3==x2','error x3==x1','Location','NorthEastOutside')
legend boxoff
title(['error event sensitivity for p' num2str(ip)])
xlabel('event #')
ylabel('sz')
box on
end
set(gcf,'Position',[100 300 1200 500])
```

3.2 Example 2

3.2.1 Model Definition

```
function [model] = example_model_2_syms()
```

CVODES OPTIONS

```
% set the default absolute tolerance
model.atol = 1e-8;
% set the default relative tolerance
model.rtol = 1e-8;
% set the default maximum number of integration steps
model.maxsteps = 1e4;
% set the parametrisation of the problem options are 'log', 'log10' and
% 'lin' (default).
model.param = 'log10';
```

STATES

```
% create state syms
syms x1 x2
% create state vector
x = [ x1 x2 ];
```

PARAMETERS (for these sensitivities will be computed)

```
% create parameter syms
syms p1 p2 p3 p4
% create parameter vector
p = [p1,p2,p3,p4];
```

SYSTEM EQUATIONS

```
% create symbolic variable for time
syms t

xdot = sym(zeros(size(x)));
% piecewise defined function
xdot(1) = -p1*x1 + dirac(t-p2);
% inhomogeneous
xdot(2) = p3*x1 - p4*x2;
```

INITIAL CONDITIONS

```
x0 = sym(zeros(size(x)));
x0(1) = 0;
x0(2) = 0;
```

OBSERVALES

```
y = sym(zeros(1,1));

y(1) = x2;
```

SYSTEM STRUCT

3.2.2 Simulation

clear

COMPILATION

3.2 Example 2 15

```
[exdir,~,~]=fileparts(which('example_model_2.m'));
% compile the model
amiwrap('model_example_2','example_model_2_syms',exdir)
Generating model struct ...
Parsing model struct ...
Generating C code ...
headers | wrapfunctions |
Compiling mex file ...
Building with 'Xcode with Clang'.
MEX completed successfully.
SIMULATION
% time vector
t = linspace(0,3,1001);
p = [1;0.5;2;3];
k = [];
options.sensi = 0;
options.cvode_maxsteps = 1e6;
\mbox{\%} load mex into memory
[msg] = which ('simulate_model_example_2'); \ % \ fix \ for \ inaccessability \ problems
sol = simulate_model_example_2(t,log10(p),k,[],options);
sol = simulate_model_example_2(t,log10(p),k,[],options);
disp(['Time elapsed with amiwrap: ' num2str(toc) ])
Time elapsed with amiwrap: 0.0019205
ODE15S
sig = 1e-2;
delta_num = @(tau) exp(-1/2*(tau/sig).^2)/(sqrt(2*pi)*sig);
ode_system = @(t,x,p,k) [-p(1)*x(1)+delta_num(t-p(2));
    +p(3)*x(1) - p(4)*x(2);
options_ode45 = odeset('RelTol', 1e-8,'AbsTol', 1e-8,'MaxStep', 1e4);
tic
[\sim, X_{ode45}] = ode45(@(t,x) ode_system(t,x,p,k),t,[0;0],options_ode45);
disp(['Time elapsed with ode45: ' num2str(toc) ])
Time elapsed with ode45: 0.042852
PLOTTING
figure
c_x = get(gca,'ColorOrder');
subplot(2,2,1)
for ix = 1:size(sol.x,2)
    plot(t,sol.x(:,ix),'.-','Color',c_x(ix,:))
    hold on
    plot(t, X_ode45(:,ix),'--','Color',c_x(ix,:))
legend('x1','x1_ode45','x2','x2_ode15s','Location','NorthEastOutside')
legend boxoff
xlabel('time t')
ylabel('x')
box on
subplot(2,2,2)
\verb"plot(t,abs(sol.x-X_ode45)",'--'")"
set(gca,'YScale','log')
ylim([1e-10,1e0])
legend('error x1','error x2','Location','NorthEastOutside')
legend boxoff
subplot(2,2,3)
plot(t,sol.y,'.-','Color',c_x(1,:))
```

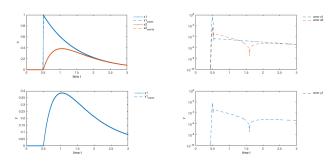
legend('y1','y1_ode45','Location','NorthEastOutside')

plot(t, X_ode45(:,2),'--','Color',c_x(1,:))

hold on

```
legend boxoff
xlabel('time t')
ylabel('y')
box on

subplot(2,2,4)
plot(t,abs(sol.y-X_ode45(:,2)),'--')
set(gca,'YScale','log')
ylim([1e-10,1e0])
legend('error y1','Location','NorthEastOutside')
legend boxoff
xlabel('time t')
ylabel('y')
box on
set(gcf,'Position',[100 300 1200 500])
```



FORWARD SENSITIVITY ANALYSIS

```
options.sensi = 1;
sol = simulate_model_example_2(t,log10(p),k,[],options);
```

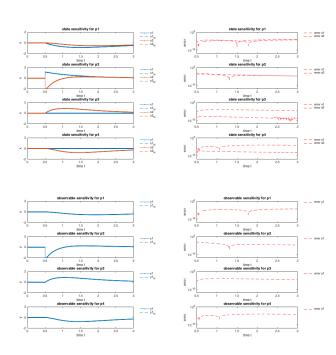
FINITE DIFFERENCES

```
eps = 1e-4;
xi = log10(p);
for ip = 1:4;
    xip = xi;
    xip(ip) = xip(ip) + eps;
    solp = simulate_model_example_2(t,xip,k,[],options);
    sx_fd(:,:,ip) = (solp.x - sol.x)/eps;
    sy_fd(:,:,ip) = (solp.y - sol.y)/eps;
end
```

```
figure
for ip = 1:4
    subplot(4,2,ip*2-1)
     hold on
     for ix = 1:size(sol.x, 2)
         plot(t,sx_fd(:,ix,ip),'.-','Color',c_x(ix,:))
plot(t,sx_fd(:,ix,ip),'.-','Color',c_x(ix,:))
     end
     ylim([-2,2])
legend('x1','x1_fd','x2','x2_fd','Location','NorthEastOutside')
     legend boxoff
     title(['state sensitivity for p' num2str(ip)])
     xlabel('time t')
     ylabel('x')
     box on
     subplot(4,2,ip*2)
    plot(t,abs(sol.sx(:,:,ip)-sx_fd(:,:,ip)),'r--')
legend('error x1','error x2','Location','NorthEastOutside')
     legend boxoff
    title(('state sensitivity for p' num2str(ip)])
xlabel('time t')
     ylabel('error')
     ylim([1e-12,1e0])
     set(gca,'YScale','log')
```

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```
box on
set(gcf,'Position',[100 300 1200 500])
figure
for ip = 1:4
     subplot (4,2,ip*2-1)
     hold on
     for iy = 1:size(sol.y, 2)
          plot(t,sq.fg(:,iy,ip),'.-','Color',c_x(iy,:))
plot(t,sy_fd(:,iy,ip),'--','Color',c_x(iy,:))
     end
     ylim([-2,2])
     legend('y1','y1_fd','Location','NorthEastOutside')
     legend boxoff
     title(['observable sensitivity for p' num2str(ip)])
xlabel('time t')
     ylabel('y')
     box on
     subplot(4,2,ip*2)
     plot(t,abs(sol.sy(:,:,ip)-sy_fd(:,:,ip)),'r--')
legend('error y1','Location','NorthEastOutside')
     legend boxoff
     regent boolf
title(['observable sensitivity for p' num2str(ip)])
xlabel('time t')
     ylabel('error')
     ylim([1e-12,1e0])
set(gca,'YScale','log')
     box on
end
set(gcf,'Position',[100 300 1200 500])
```



3.3 Example 3

3.3.1 Model Definition

```
function [model] = example_model_3_syms()
```

CVODES OPTIONS

```
\$ set the default absolute tolerance model.atol = 1e-8; \$ set the default relative tolerance model.rtol = 1e-8; \$ set the default maximum number of integration steps model.maxsteps = 1e4;
```

```
\$ set the parametrisation of the problem options are 'log', 'log10' and \$ 'lin' (default). model.param = 'log10';
```

STATES

```
% create state syms
syms x1 x2 x3
% create state vector
x = [
x1 x2 x3
];
```

PARAMETERS (for these sensitivities will be computed)

```
% create parameter syms
syms p1 p2 p3 p4 p5
% create parameter vector
p = [p1,p2,p3,p4,p5];
```

CONSTANTS (for these no sensitivities will be computed) this part is optional and can be ommitted

```
% create parameter syms
syms k1 k2 k3 k4
% create parameter vector
k = [k1 k2 k3 k4];
```

SYSTEM EQUATIONS

```
% create symbolic variable for time
syms t

xdot = sym(zeros(size(x)));
% piecewise defined function
xdot(1) = -2*p1*x1^2 - p2*x1*x2 + 2*p3*x2 + p4*x3 + p5;
% inhomogeneous
xdot(2) = +p1*x1^2 - p2*x1*x2 - p3*x2 + p4*x3;
xdot(3) = p2*x1*x2 - p4*x(3) - k4*x(3);
```

INITIAL CONDITIONS

```
x0 = sym(zeros(size(x)));
x0(1) = k1;
x0(2) = k2;
x0(3) = k3;
```

OBSERVALES

```
y = sym(zeros(1,1));

y = x;
```

SYSTEM STRUCT

```
model.sym.x = x;
model.sym.k = k;
model.sym.xdot = xdot;
model.sym.p = p;
model.sym.x0 = x0;
model.sym.y = y;
```

3.3 Example 3 19

3.3.2 Simulation

clear

COMPILATION

```
[exdir,~,~]=fileparts(which('example_model_3.m'));
% compile the model
amiwrap('model_example_3','example_model_3_syms',exdir)
% add the model to the path
addpath(genpath([strrep(which('amiwrap.m'),'amiwrap.m','') 'models/model_example_3']))

Generating model struct ...
Parsing model struct ...
Generating C code ...
headers | wrapfunctions |
Compiling mex file ...
Building with 'Xcode with Clang'.
MEX completed successfully.
```

SIMULATION

```
% time vector
t = linspace(0,300,20);
p = [1;0.5;0.4;2;0.1];
k = [0.1,0.4,0.7,1];

options.sensi = 0;
options.cvode_maxsteps = 1e6;
% load mex into memory
sol = simulate_model_example_3(t,log10(p),k,[],options);

tic
sol = simulate_model_example_3(t,log10(p),k,[],options);
disp(['Time elapsed with cvodes: ' num2str(toc) ])
```

ODE15S

Time elapsed with cvodes: 0.002146

```
figure
c_x = get(gca,'ColorOrder');
subplot(2,2,1)
for ix = 1:size(sol.x,2)
    plot(t,sol.x(:,ix),'.-','Color',c_x(ix,:))
    hold on
```

```
plot(t,X_odel5s(:,ix),'d','Color',c_x(ix,:))
end
legend('x1','x1_odel5s','x2','x2_odel5s','x3','x3_odel5s','Location','NorthEastOutside')
legend boxoff
xlabel('time t')
ylabel('x')
box on
subplot(2,2,2)
plot(t,abs(sol.x-X_odel5s),'--')
set(gca,'YScale','log')
legend('error x1','error x2','error x3','Location','NorthEastOutside')
legend boxoff
set(gcf,'Position',[100 300 1200 500])
```

FORWARD SENSITIVITY ANALYSIS

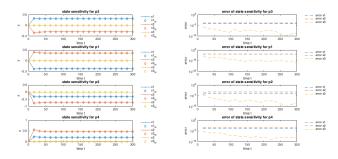
```
options.sensi = 1;
options.sens_ind = [3,1,2,4];
sol = simulate_model_example_3(t,log10(p),k,[],options);
```

FINITE DIFFERENCES

```
eps = 1e-3;
xi = log10(p);
for ip = 1:4;
    xip = xi;
    xip(ip) = xip(ip) + eps;
    solp = simulate_model_example_3(t,xip,k,[],options);
    sx_fd(:,:,ip) = (solp.x - sol.x)/eps;
    sy_fd(:,:,ip) = (solp.y - sol.y)/eps;
end
```

```
figure
for ip = 1:4
    subplot(4,2,ip*2-1)
    hold on
    for ix = 1:size(sol.x, 2)
         plot(t, sol.sx(:,ix,ip),'.-','Color',c_x(ix,:))
         plot(t, sx_fd(:,ix,options.sens_ind(ip)),'d','Color',c_x(ix,:))
    \texttt{legend('x1','x1\_fd','x2','x2\_fd','x3','x3\_fd','Location','NorthEastOutside')}
    legend boxoff
title(['state sensitivity for p' num2str(options.sens_ind(ip))])
    xlabel('time t')
    ylabel('x')
    subplot(4,2,ip*2)
    plot(t,abs(sol.sx(:,:,ip)-sx_fd(:,:,options.sens_ind(ip))),'--')
legend('error x1','error x2','error x3','Location','NorthEastOutside')
    legend boxoff
    title(['error of state sensitivity for p' num2str(options.sens_ind(ip))])
    xlabel('time t')
    ylabel('error')
    set(gca,'YScale','log')
    box on
set(gcf,'Position',[100 300 1200 500])
```

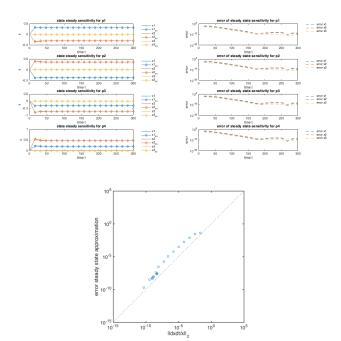
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STEADY STATE SENSITIVITY

```
sssens = NaN(size(sol.sx));
for it = 2:length(t)
    tt = [0,t(it)];
    options.sensi_meth = 'ss';
    solss = simulate_model_example_3(tt,log10(p),k,[],options);
    sssens(it,:,:) = solss.sx;
    ssxdot(it,:) = solss.xdot;
end
```

```
figure
for ip = 1:4
     subplot(4,2,ip*2-1)
     hold on
     for ix = 1:size(sol.x, 2)
          plot(t,ssens(:,ix,ip),'.-','Color',c_x(ix,:))
plot(t,ssens(:,ix,ip),'d-','Color',c_x(ix,:))
     end
     legend('x1','x1_ss','x2','x2_ss','x3','x3_ss','Location','NorthEastOutside')
     legend boxoff
     title(['state steady sensitivity for p' num2str(ip)])
xlabel('time t')
     ylabel('x')
     box on
     subplot(4,2,ip*2)
     plot(t,abs(sol.sx(:,:,ip))-sssens(:,:,ip)),'--')
legend('error x1','error x2','error x3','Location','NorthEastOutside')
     legend boxoff
     title(['error of steady state sensitivity for p' num2str(ip)])
     xlabel('time t')
     ylabel('error')
     set(gca,'YScale','log')
     box on
end
set(gcf,'Position',[100 300 1200 500])
\verb|scatter(sqrt(sum((ssxdot./sol.x).^2,2)),sqrt(sum((sol.sx-sssens).^2,2),3))||
hold on
plot([1e-15,1e5],[1e-15,1e5],'k:')
set(gca,'YScale','log')
set(gca,'XScale','log')
box on
xlabel('||dxdt/x||_2')
ylabel('error steady state approximation')
set (gca, 'FontSize', 15)
set (gca, 'LineWidth', 1.5)
set(gcf,'Position',[100 300 1200 500])
```



3.4 Example 4

3.4.1 Model Definition

```
function [model] = example_model_4_syms()
```

CVODES OPTIONS

```
model.ato1 = 1e-12;
model.rto1 = 1e-8;
model.maxsteps = 1e4;
model.param = 'log10';
```

STATES

PARAMETERS

```
syms p1 p2 p3 p4 init_STAT Omega_cyt Omega_nuc sp1 sp2 sp3 sp4 sp5 offset_tSTAT offset_pSTAT scale_tSTAT scale_pSTAT scale_pSTAT sigma_pSTAT, sigma_pSTAT, sigma_pSTAT, sigma_tSTAT, s
```

INPUT

```
syms t u(1) = spline_pos5(t, 0.0, sp1, 5.0, sp2, 10.0, sp3, 20.0, sp4, 60.0, sp5, 0, 0.0);
```

SYSTEM EQUATIONS

3.4 Example 4 23

```
xdot = sym(zeros(size(x)));

xdot(1) = (Omega_nuc*p4*nSTAT5 - Omega_cyt*STAT*p1*u(1))/Omega_cyt;
xdot(2) = STAT*p1*u(1) - 2*p2*pSTAT^2;
xdot(3) = p2*pSTAT^2 - p3*pSTAT_pSTAT;
xdot(4) = -(Omega_nuc*p4*npSTAT_npSTAT - Omega_cyt*p3*pSTAT_pSTAT)/Omega_nuc;
xdot(5) = -p4*(nSTAT1 - 2*npSTAT_npSTAT);
xdot(6) = p4*(nSTAT1 - nSTAT2);
xdot(7) = p4*(nSTAT2 - nSTAT3);
xdot(8) = p4*(nSTAT3 - nSTAT4);
xdot(9) = p4*(nSTAT4 - nSTAT5);
```

INITIAL CONDITIONS

```
x0 = sym(zeros(size(x)));
x0(1) = init STAT;
```

OBSERVABLES

```
y = sym(zeros(3,1));

y(1) = offset_pSTAT + scale_pSTAT/init_STAT*(pSTAT + 2*pSTAT_pSTAT);
y(2) = offset_tSTAT + scale_tSTAT/init_STAT*(STAT + pSTAT + 2*(pSTAT_pSTAT));
y(3) = u(1);
```

SIGMA

```
sigma_y = sym(size(y));
sigma_y(1) = sigma_pSTAT;
sigma_y(2) = sigma_tSTAT;
sigma_y(3) = sigma_pEpoR;
```

SYSTEM STRUCT

```
model.sym.x = x;
model.sym.u = u;
model.sym.xdot = xdot;
model.sym.p = p;
model.sym.k = k;
model.sym.x0 = x0;
model.sym.y = y;
model.sym.sigma_y = sigma_y;

end

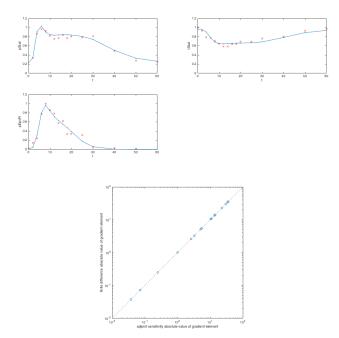
ans =
    atol: le-12
    rtol: le-08
    maxsteps: 10000
    param: 'log10'
    sym: [lx1 struct]
```

3.4.2 Simulation

```
clear
% compile the model
[exdir,~,~]=fileparts(which('example_model_4.m'));
amiwrap('model_example_4','example_model_4_syms',exdir)
num = xlsread(fullfile(exdir,'pnas_data_original.xls'));
t = num(:,1);
D.Y = num(:,[2,4,6]);
D.Sigma_Y = NaN(size(D.Y));
```

```
kappa = [1.4, 0.45];
xi = [0.595102743982229]
    2.9999999999997
    -0.948930681736172
    -0.00751433662124028
    -2.78593598707493
    -0.256066441623149
    -0.07511250551843
    -0.411247187909784
    -4.9999999959546
    -0.735327875726678
    -0.64146041506584
    -0.107897525629158
    0.0272647740863191
    -0.5
    0
    -0.5];
options.sensi = 0;
sol = simulate_model_example_4(t,xi,kappa,D,options);
figure
for iy = 1:3
    subplot(2,2,iy)
    plot(t,D.Y(:,iy),'rx')
    hold on
    plot(t, sol.y(:, iy),'.-')
    xlim([0,60])
    xlabel('t')
    switch(iy)
        case 1
            ylabel('pStat')
         case 2
        ylabel('tStat')
case 3
            ylabel('pEpoR')
    ylim([0,1.2])
end
set(gcf,'Position',[100 300 1200 500])
% generate new
xi_rand = xi + 0.1;
options.sensi = 1;
options.sensi_meth = 'adjoint';
sol = simulate_model_example_4(t,xi_rand,kappa,D,options);
options.sensi = 0;
eps = 1e-4;
fd_grad = NaN(length(xi),1);
for ip = 1:length(xi)
xip = xi_rand;
    xip(ip) = xip(ip) + eps;
psol = simulate_model_example_4(t,xip,kappa,D,options);
    fd_grad(ip) = (psol.llh-sol.llh)/eps;
figure
scatter(abs(sol.sllh),abs(fd grad))
set (gca, 'XScale', 'log')
set (gca, 'YScale', 'log')
xlim([1e-2,1e2])
ylim([1e-2,1e2])
box on
hold on
axis square
plot([1e-2,1e2],[1e-2,1e2],'k:')
xlabel('adjoint sensitivity absolute value of gradient element')
ylabel('finite difference absolute value of gradient element')
set(gcf,'Position',[100 300 1200 500])
Generating model struct ...
Parsing model struct ...
Generating C code ...
headers | wrapfunctions |
Compiling mex file ...
Building with 'Xcode with Clang'.
MEX completed successfully.
```

3.5 Example 5 25



3.5 Example 5

3.5.1 Model Definition

```
function [model] = example_model_5_syms()
```

CVODES OPTIONS

```
% set the default absolute tolerance
model.atol = 1e-8;
% set the default relative tolerance
model.rtol = 1e-8;
% set the default maximum number of integration steps
model.maxsteps = 1e4;
% set the parametrisation of the problem options are 'log', 'log10' and
% 'lin' (default).
model.param = 'log10';
```

STATES

```
% create state syms
syms x1 x2
% create state vector
x = [ x1 x2 ];
```

PARAMETERS (for these sensitivities will be computed)

```
% create parameter syms
syms p1 p2 p3 p4
% create parameter vector
p = [p1,p2,p3,p4];
```

SYSTEM EQUATIONS

```
\mbox{\ensuremath{\mbox{\$}}} create symbolic variable for time syms t
```

```
xdot = sym(zeros(size(x)));
% piecewise defined function
xdot(1) = -p1*x1 + dirac(t-p2);
% inhomogeneous
xdot(2) = p3*x1 - p4*x2;
```

INITIAL CONDITIONS

```
x0 = sym(zeros(size(x)));
x0(1) = 0;
x0(2) = 0;
```

OBSERVALES

```
y = sym(zeros(1,1));

y(1) = x2;
```

SYSTEM STRUCT

3.5.2 Simulation

clear

COMPILATION

```
[exdir,~,~]=fileparts(which('example_model_5.m'));
% compile the model
amiwrap('model_example_5','example_model_5_syms',exdir)

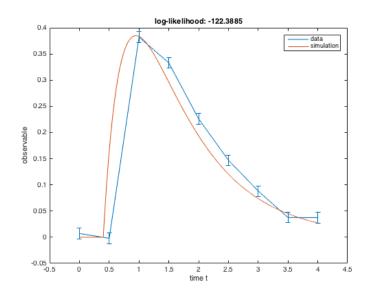
Generating model struct ...
Parsing model struct ...
Generating C code ...
headers | wrapfunctions |
Compiling mex file ...
Building with 'Xcode with Clang'.
MEX completed successfully.
```

SIMULATION

```
% time vector
tout = linspace(0,4,9);
tfine = linspace(0,4,10001);
p = [1;0.4;2;3];
k = [];
D.Y = [ 0.00714742903826096
```

3.5 Example 5 27

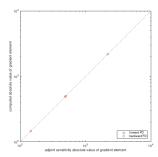
```
-0.00204966058299775
          0.382159034587845
           0.33298932672138
          0.226111476113441
          0.147028440865854
         0.0882468698791813
         0.0375887796628869
         0.0373422340295005];
D.Sigma_Y = 0.01*ones(size(D.Y));
options.sensi = 1;
options.sensi_meth = 'adjoint';
options.cvode_maxsteps = 1e4;
sol = simulate_model_example_5(tout,log10(p),k,D,options);
options.sensi = 0;
solfine = simulate_model_example_5(tfine, log10(p), k, [], options);
figure
errorbar(tout, D.Y, D.Sigma_Y)
hold on
plot(tfine, solfine.y)
legend('data', 'simulation')
xlabel('time t')
ylabel('observable')
title(['log-likelihood: ' num2str(sol.llh) ])
```



FD

```
eps = 1e-4;
xi = log10(p);
grad_fd_f = NaN(4,1);
grad_fd_b = NaN(4,1);
for ip = 1:4;
     options.sensi = 0;
     xip = xi;
     xip(ip) = xip(ip) + eps;
     solpf = simulate_model_example_5(tout,xip,k,D,options);
     grad_fd_f(ip,1) = (solpf.llh-sol.llh)/eps;
     xip = xi;
xip(ip) = xip(ip) - eps;
solpb = simulate_model_example_5(tout,xip,k,D,options);
     grad_fd_b(ip,1) = -(solpb.llh-sol.llh)/eps;
end
figure
plot(abs(grad_fd_f),abs(sol.sllh),'o')
hold on
plot (abs(grad_fd_b), abs(sol.sllh),'o')
set (gca, 'XScale', 'log')
set (gca, 'YScale', 'log')
hold on
axis square
plot([1e2,1e4],[1e2,1e4],'k:')
xlim([1e2,1e4])
```

```
ylim([le2,1e4])
legend('forward FD','backward FD','Location','SouthEast')
xlabel('adjoint sensitivity absolute value of gradient element')
ylabel('computed absolute value of gradient element')
set(gcf,'Position',[100 300 1200 500])
```



3.6 Example 6

3.6.1 Model Definition

```
function [model] = example_model_6_syms()
```

CVODES OPTIONS

```
% set the default absolute tolerance
model.atol = 1e-8;
% set the default relative tolerance
model.rtol = 1e-8;
% set the default maximum number of integration steps
model.maxsteps = 1e4;
% set the parametrisation of the problem options are 'log', 'log10' and
% 'lin' (default).
model.param = 'log10';
```

STATES

```
% create state syms
syms x1
% create state vector
x = [ x1];
```

PARAMETERS (for these sensitivities will be computed)

```
% create parameter syms
syms p1 p2 p3
% create parameter vector
p = [p1 p2 p3];
```

SYSTEM EQUATIONS

```
% create symbolic variable for time
syms t

xdot = sym(zeros(size(x)));
% piecewise defined function
xdot(1) = -p1*x1*heaviside(t-2) + p2;
```

INITIAL CONDITIONS

3.6 Example 6 29

```
x0 = sym(zeros(size(x)));
x0(1) = p3;
```

OBSERVALES

```
y = sym(zeros(1,1));

y(1) = x1;
```

SYSTEM STRUCT

```
model.sym.x = x;
model.sym.xdot = xdot;
model.sym.p = p;
model.sym.x0 = x0;
model.sym.y = y;

end

ans =
    atol: le-08
    rtol: le-08
    maxsteps: 10000
    param: 'log10'
    sym: [1x1 struct]
```

3.6.2 Simulation

clear

COMPILATION

```
[exdir,~,~]=fileparts(which('example_model_6.m'));
% compile the model
amiwrap('model_example_6','example_model_6_syms',exdir)

Generating model struct ...
Parsing model struct ...
Generating C code ...
headers | wrapfunctions |
Compiling mex file ...
Building with 'Xcode with Clang'.
MEX completed successfully.
```

SIMULATION

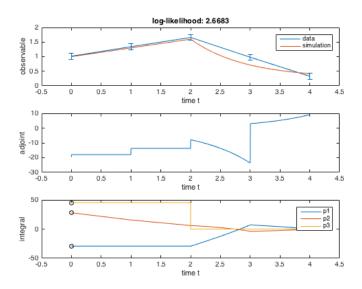
```
% time vector
t = [linspace(0,4,5)];
p = [1.1,0.3,1];
k = [];
% D.Y = [
% 1.1761
               1.0171
      1.1680
      1.1359
      1.1778
      1.3423
      1.3079
      1.2784
      1.4976
      1.5903
      1.6585
      1.4688
      1.0999
      1.0128
      0.7198
      0.9814
      0.6755
```

```
0.5091
      0.4471
용
      0.5249
용
      0.32881;
D.Y = [
           1.0171
    1.3423
    1.6585
    0.9814
    0.32881;
D.Sigma_Y = 0.1*ones(size(D.Y));
options.sensi = 1;
options.sensi_meth = 'adjoint';
options.cvode_maxsteps = 1e6;
options.cvode_rtol = 1e-12;
options.cvode_atol = 1e-12;
% load mex into memory
[msg] = which('simulate_model_example_6'); % fix for inaccessability problems
sol = simulate_model_example_6(t,log10(p),k,D,options);
```

Plot

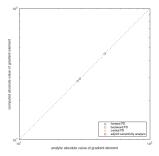
```
figure
 subplot(3,1,1)
 errorbar(t,D.Y,D.Sigma_Y)
hold on
% plot(t,sol.y)
xlabel('time t')
ylabel('observable')
title(['log-likelihood: ' num2str(sol.llh) ])
v = (p(2) *t + p(3)) *(t < 2) + ((2*p(2) + p(3) - p(2) / p(1)) *exp(-p(1) *(t-2)) + p(2) / p(1)) *(t > = 2);
tfine = linspace(0,4,100001);
 \texttt{xfine} = (\texttt{p(2)} * \texttt{tfine} + \texttt{1)} . * (\texttt{tfine} < \texttt{2}) + ((2*\texttt{p(2)} + \texttt{p(3)} - \texttt{p(2)} / \texttt{p(1)}) * \texttt{exp(-p(1)} * (\texttt{tfine} - \texttt{2})) + \texttt{p(2)} / \texttt{p(1)}) . * (\texttt{tfine} > = \texttt{2}); 
mu = zeros(1,length(tfine));
for it = 1:length(t)
 if(t(it)<=2)
mu = mu + ((y(it)-D.Y(it))/(D.Sigma_Y(it)^2))*(tfine <= t(it));
else
 \texttt{mu} = \texttt{mu} + ((\texttt{y(it)} - \texttt{D.Y(it)}) / (\texttt{D.Sigma\_Y(it)} ^2)) \\ \star \texttt{exp}(\texttt{p(1)} \star (\texttt{tfine-t(it)})) \\ \star (\texttt{tfine-t(it)})) \\ \star (\texttt{tfine-t(it)}) \\ \star (
end
end
plot(tfine, xfine)
legend('data','simulation')
xlim([min(t)-0.5,max(t)+0.5])
subplot(3,1,2)
plot(tfine.mu)
ylabel('adjoint')
xlabel('time t')
xlim([min(t)-0.5, max(t)+0.5])
subplot(3,1,3)
\verb|plot(fliplr(tfine),-cumsum(fliplr(-mu.*xfine.*(tfine>2)))*p(1)*log(10)*(t(end)/numel(tfine))||
hold on
\verb|plot(flip|r(tfine),-cumsum(flip|r(mu))*p(2)*log(10)*(t(end)/numel(tfine))||\\
\verb|plot(tfine,-mu(1)*p(3)*log(10)*(tfine<2)||
 xlim([min(t)-0.5, max(t)+0.5])
ylabel('integral')
xlabel('time t')
legend('p1','p2','p3')
grad(1,1) = -trapz(tfine, -mu.*xfine.*(tfine>2))*p(1)*log(10);
grad(2,1) = -trapz(tfine,mu)*p(2)*log(10);
grad(3,1) = -mu(1)*p(3)*log(10);
plot(zeros(3,1),grad,'ko')
```

3.6 Example 6 31



FD

```
eps = 1e-5;
xi = log10(p);
grad_fd_f = NaN(3,1);
grad_fd_b = NaN(3,1);
for ip = 1:3;
    options.sensi = 0;
    xip = xi;
    xip(ip) = xip(ip) + eps;
       solp = simulate_model_example_6(t,xip,k,D,options);
       grad_fd_f(ip,1) = (solp.llh-sol.llh)/eps;
       xip = xi;
       xip(ip) = xip(ip) - eps;
       salp(ip) = Aip(ip) eps,
solp = simulate_model_example_6(t,xip,k,D,options);
grad_fd_b(ip,1) = -(solp.llh-sol.llh)/eps;
figure
plot(abs(grad),abs(grad_fd_f),'o')
hold on
plot (abs(grad), abs(grad_fd_b),'o')
plot (abs(grad), mean([abs(grad_fd_b), abs(grad_fd_f)],2),'o')
plot (abs(grad), abs(sol.sllh),'o')
plot([le1,1e2],[le1,1e2],'k:')
set(gca,'XScale','log')
set(gca,'YScale','log')
axis square
axis square legend('forward FD','backward FD','central FD','adjoint sensintivity analysis','Location','SouthEast') xlabel('analytic absolute value of gradient element') ylabel('computed absolute value of gradient element') set(gcf,'Position',[100 300 1200 500])
```



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 Hierarchical Index

5.1 Class Hierarchy

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

amievent	37
amifun	39
ExpData	64
funTest handle	65
amidata	34
amimodel	44
SBMLode SetGet	69
amioption	60
modelTest	65

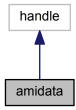
6 Class Index 33

	ReturnData sym	67
	optsym	66
	TempData	74
	UserData	81
ŝ	Class Index	
,	Oldos Illuck	
3.1	Class List	
Нe	re are the classes, structs, unions and interfaces with brief descriptions:	
	amidata AMIDATA provides a data container to pass experimental data to the simulation routine for likelihood computation	34
	amievent Amievent class defines the prototype for all events which later on will be transformed into C code	37
	amifun Amifun class defines the prototype for all functions which later on will be transformed into C code	39
	amimodel Amimodel is the object in which all model definitions are stored	44
	amioption AMIOPTION provides an option container to pass simulation parameters to the simulation routine	60
	ExpData Struct that carries all information about experimental data	64
	funTest FUNTEST Summary of this class goes here Detailed explanation goes here	65
	modelTest MODELTEST Summary of this class goes here Detailed explanation goes here	65
	optsym OPTSYM is a placeholder class to get access to the protected sym.s	66
	ReturnData Struct that stores all data which is later returned by the mex function	67
	SBMLode SBMLODE carries all information about the differential equation defined by a SBML model definition file. This class acts as an interface between SBML files and amimodel	69
	TempData Struct that provides temporary storage for different variables	74
	UserData Struct that stores all user provided data	81

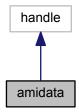
7 Class Documentation

7.1 amidata Class Reference

AMIDATA provides a data container to pass experimental data to the simulation routine for likelihood computation. Inheritance diagram for amidata:



Collaboration diagram for amidata:



Public Member Functions

 amidata (matlabtypesubstitute varargin) initialisation via struct

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("[]")
        timepoints of observations
    matlabtypesubstitute Y = double("[]")
        observations
    matlabtypesubstitute Sigma_Y = double("[]")
        standard deviation of observations
    matlabtypesubstitute Z = double("[]")
        event observations
    matlabtypesubstitute Sigma_Z = double("[]")
        standard deviation of event observations
```

• matlabtypesubstitute condition = double("[]")

7.1.1 Detailed Description

Definition at line 17 of file amidata.m.

experimental condition

7.1.2 Member Data Documentation

7.1.2.1 nt = 0

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 28 of file amidata.m.

7.1.2.2 ny = 0

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 36 of file amidata.m.

7.1.2.3 nz = 0

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 44 of file amidata.m.

7.1.2.4 ne = 0

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 52 of file amidata.m.

7.1.2.5 nk = 0

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 60 of file amidata.m.

7.1.2.6 t = double("[]")

Default: double("[]")

Note

This property has custom functionality when its value is changed.

Definition at line 68 of file amidata.m.

7.1.2.7 Y = double("[]")

Default: double("[]")

Note

This property has custom functionality when its value is changed.

Definition at line 76 of file amidata.m.

7.1.2.8 Sigma_Y = double("[]")

Default: double("[]")

Note

This property has custom functionality when its value is changed.

Definition at line 84 of file amidata.m.

7.1.2.9 Z = double("[]")

Default: double("[]")

Note

This property has custom functionality when its value is changed.

Definition at line 92 of file amidata.m.

```
7.1.2.10 Sigma_Z = double("[]")
```

Default: double("[]")

Note

This property has custom functionality when its value is changed.

Definition at line 100 of file amidata.m.

```
7.1.2.11 condition = double("[]")
```

Default: double("[]")

Note

This property has custom functionality when its value is changed.

Definition at line 108 of file amidata.m.

7.2 amievent Class Reference

the amievent class defines the prototype for all events which later on will be transformed into C code

Public Member Functions

- amievent (::symbolic trigger,::symbolic bolus,::symbolic z)
 constructor of the amievent class. this function constructs an event object based on the provided trigger function, bolus function and output function
- mlhsInnerSubst< matlabtypesubstitute > setHflag (::double hflag) gethflag sets the hflag property.

Public Attributes

• ::symbolic trigger = sym("[]")

the trigger function activates the event on every zero crossing

• ::symbolic bolus = sym("[]")

the bolus function defines the change in states that is applied on every event occurence

- ::symbolic **z** = sym("[]")
 - output function for the event
- ::logical hflag = logical("[]")

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

7.2.1 Detailed Description

Definition at line 17 of file amievent.m.

7.2.2 Constructor & Destructor Documentation

7.2.2.1 amievent (::symbolic trigger, ::symbolic bolus, ::symbolic z)

Parameters

trigger	trigger fuction, the roots of this function define the occurence of the event
bolus	bolus fuction, this function defines the change in the states on event occurences
Z	output function, this expression is evaluated on event occurences and returned by the simu-
	lation function

Definition at line 75 of file amievent.m.

7.2.3 Member Function Documentation

7.2.3.1 mlhslnnerSubst<::amievent > setHflag (::double hflag)

Parameters

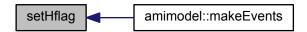
hflag	value for the hflag property

Return values

this	updated event definition object

Definition at line 18 of file setHflag.m.

Here is the caller graph for this function:



7.2.4 Member Data Documentation

7.2.4.1 trigger = sym("[]")

Note

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

Matlab documentation of property attributes.

Default: sym("[]")

Definition at line 27 of file amievent.m.

7.2.4.2 bolus = sym("[]")

Note

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

Matlab documentation of property attributes.

Default: sym("[]")

Definition at line 38 of file amievent.m.

7.2.4.3 z = sym("[]")

Note

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

Default: sym("[]")

Definition at line 49 of file amievent.m.

7.2.4.4 hflag = logical("[]")

Note

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

Matlab documentation of property attributes.

Default: logical("[]")

Definition at line 60 of file amievent.m.

7.3 amifun Class Reference

the amifun class defines the prototype for all functions which later on will be transformed into C code

Public Member Functions

• amifun (::string funstr,::amimodel model)

constructor of the amifun class. this function initializes the function object based on the provided function name funstr and model definition object model

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 gccode (::amimodel model,::fileid fid)

gccode transforms symbolic expressions into c code and writes the respective expression into a specified file

mlhsInnerSubst< matlabtypesubstitute > getDeps (::amimodel model)

getDeps populates the sensiflag for the requested function

mlhsInnerSubst< matlabtypesubstitute > getArgs (::amimodel model)

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

mlhsInnerSubst< matlabtypesubstitute > getFArgs (::amimodel model)

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_{ν} 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

mlhslnnerSubst< matlabtypesubstitute > getSyms (::amimodel model)

getSyms computes the symbolic expression for the requested function

mlhsInnerSubst< matlabtypesubstitute > getSensiFlag ()

getSensiFlag populates the sensiflag property

Public Attributes

• ::symbolic sym

symbolic definition struct

· ::symbolic strsym

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

• ::symbolic strsym_old

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

· ::char funstr

name of the model

• ::char cvar

name of the c variable

· ::char argstr

argument string (solver specific)

· ::char fargstr

argument string (solver unspecific)

• ::cell deps

dependencies on other functions

• ::cell nvecs

nvec dependencies

::logical sensiflag

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

7.3.1 Detailed Description

Definition at line 17 of file amifun.m.

7.3.2 Constructor & Destructor Documentation

7.3.2.1 amifun (::string funstr, ::amimodel model)

Parameters

funstr	name of the function
model	model definition object

Definition at line 101 of file amifun.m.

7.3.3 Member Function Documentation

7.3.3.1 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.

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

Parameters

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

Return values

fid	void

Definition at line 18 of file writeCcode_sensi.m.

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

Parameters

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

Return values

fid	void

Definition at line 18 of file writeCcode.m.

Here is the call graph for this function:



7.3.3.4 mlhslnnerSubst<::amifun > gccode (::amimodel model, ::fileid fid)

Parameters

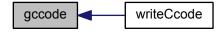
model	model defintion object
fid	file id in which the expression should be written

Return values

this	function definition object

Definition at line 18 of file gccode.m.

Here is the caller graph for this function:



7.3.3.5 mlhslnnerSubst<:::amifun > getDeps (::amimodel model)

Parameters

model | model definition object

Return values

this updated function definition object

Definition at line 18 of file getDeps.m.

7.3.3.6 mlhslnnerSubst<::amifun > getArgs (::amimodel model)

Parameters

model | model definition object

Return values

this updated function definition object

Definition at line 18 of file getArgs.m.

7.3.3.7 mlhslnnerSubst<::amifun > getFArgs (::amimodel model)

Parameters

model | model definition object

Return values

this updated function definition object

Definition at line 18 of file getFArgs.m.

7.3.3.8 mlhslnnerSubst<::amifun > getNVecs ()

Return values

this updated function definition object

Definition at line 18 of file getNVecs.m.

7.3.3.9 mlhslnnerSubst<::amifun > getCVar ()

Return values

this updated function definition object

Definition at line 18 of file getCVar.m.

7.3.3.10 mlhsSubst< mlhsInnerSubst<:::amifun >,mlhsInnerSubst<:::amimodel >> getSyms (::amimodel model)

Parameters

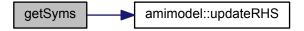
model model definition object

Return values

this	updated function definition object
model	updated model definition object

Definition at line 18 of file getSyms.m.

Here is the call graph for this function:



7.3.3.11 mlhslnnerSubst<::amifun > getSensiFlag ()

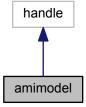
Return values

this	updated function definition object

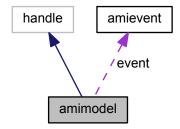
Definition at line 18 of file getSensiFlag.m.

7.4 amimodel Class Reference

amimodel is the object in which all model definitions are stored Inheritance diagram for amimodel:



Collaboration diagram for amimodel:



Public Member Functions

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

constructor of the amimodel class. this function initializes the model object based on the provided symfun and modelname

noret::substitute updateRHS (::sym xdot)

updateRHS updates the right hand side of the model

• 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.

Public Attributes

· ::struct sym

symbolic definition struct

::struct fun

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

name of the model

· ::struct HTable

struct that contains hash values for the symbolic model definitions

• ::double atol = 1e-8

default absolute tolerance

• ::double rtol = 1e-8

default relative tolerance

• ::int maxsteps = 1e4

default maximal number of integration steps

• ::logical debug = false

flag indicating whether debugging symbols should be compiled

• ::logical adjoint = true

flag indicating whether adjoint sensitivities should be enabled

• ::logical forward = true

flag indicating whether forward sensitivities should be enabled

• ::double t0 = 0

default initial time

· ::char wtype

type of wrapper (cvodes/idas)

::int nx

number of states

• ::int nxtrue = 0

number of original states for second order sensitivities

• ::int ny

number of observables

• ::int nytrue = 0

number of original observables for second order sensitivities

::int np

number of parameters

::int nk

number of constants

· ::int nevent

number of events

::int nz

number of event outputs

· ::int nztrue

number of original event outputs for second order sensitivities

::*int id

flag for DAEs

• ::int ubw

upper Jacobian bandwidth

• ::int lbw

lower Jacobian bandwidth

· ::int nnz

number of nonzero entries in Jacobian

::*int sparseidx

dataindexes of sparse Jacobian

::*int rowvals

rowindexes of sparse Jacobian

::*int colptrs

columnindexes of sparse Jacobian

::*int sparseidxB

dataindexes of sparse Jacobian

::*int rowvalsB

rowindexes of sparse Jacobian

::*int colptrsB

columnindexes of sparse Jacobian

· ::cell funs

cell array of functions to be compiled

• ::char coptim = "-O3"

optimisation flag for compilation

::string param = "lin"

default parametrisation

· matlabtypesubstitute wrap_path

path to wrapper

• matlabtypesubstitute recompile = false

flag to enforce recompilation of the model

matlabtypesubstitute cfun = struct("[]")

storage for flags determining recompilation of individual functions

• matlabtypesubstitute o2flag = 0

flag which identifies augmented models 0 indicates no augmentation 1 indicates augmentation by first order sensitivities (yields second order sensitivities) 2 indicates augmentation by one linear combination of first order sensitivities (yields hessian-vector product)

• matlabtypesubstitute compver = 6

counter that allows enforcing of recompilation of models after code changes

matlabtypesubstitute z2event = double("[]")

vector that maps outputs to events

matlabtypesubstitute splineflag = false

flag indicating whether the model contains spline functions

• matlabtypesubstitute minflag = false

flag indicating whether the model contains min functions

matlabtypesubstitute maxflag = false

flag indicating whether the model contains max functions

• ::int nw = 0

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

• ::int ndwdx = 0

number of derivatives of derived variables w, dwdx

• ::int ndwdp = 0

number of derivatives of derived variables w, dwdp

7.4.1 Detailed Description

Definition at line 17 of file amimodel.m.

7.4.2 Constructor & Destructor Documentation

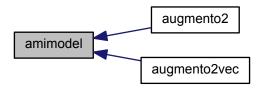
7.4.2.1 amimodel (::string symfun, ::string modelname)

Parameters

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

Definition at line 517 of file amimodel.m.

Here is the caller graph for this function:



7.4.3 Member Function Documentation

7.4.3.1 noret::substitute updateRHS (::sym xdot)

Parameters

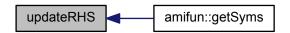
xdot	new right hand side

Return values

this	udpated model definition object

Definition at line 591 of file amimodel.m.

Here is the caller graph for this function:



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

Parameters

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

Definition at line 18 of file generateM.m.

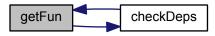
7.4.3.3 noret::substitute getFun (::struct HTable, ::string funstr)

Parameters

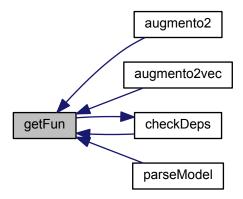
HTable	struct with hashes of symbolic definition from the previous compilation
funstr	function for which symbolic expressions should be computed

Definition at line 18 of file getFun.m.

Here is the call graph for this function:



Here is the caller graph for this function:



7.4.3.4 mlhslnnerSubst<::logical > checkDeps (::struct HTable, ::cell deps)

Parameters

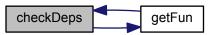
HTable	struct with reference hashes of functions in its fields
deps	cell array with containing a list of dependencies

Return values

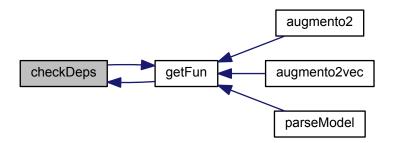
cflag	boolean indicating whether any of the dependencies have changed with respect
	to the hashes stored in HTable

Definition at line 18 of file checkDeps.m.

Here is the call graph for this function:



Here is the caller graph for this function:



7.4.3.5 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:



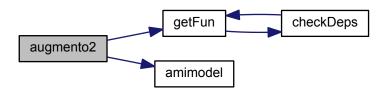
7.4.3.6 mlhsInnerSubst < matlabtypesubstitute > augmento2 ()

Return values

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

Definition at line 18 of file augmento2.m.

Here is the call graph for this function:



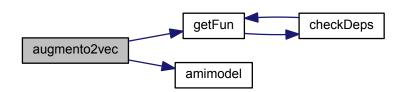
7.4.3.7 mlhslnnerSubst< matlabtypesubstitute > augmento2vec ()

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:



7.4.4 Member Data Documentation

7.4.4.1 sym

Note

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

Matlab documentation of property attributes.

Definition at line 27 of file amimodel.m.

7.4.4.2 fun

Note

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

Matlab documentation of property attributes.

Definition at line 37 of file amimodel.m.

7.4.4.3 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 47 of file amimodel.m.

7.4.4.4 modelname

Note

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

Matlab documentation of property attributes.

Definition at line 59 of file amimodel.m.

7.4.4.5 HTable

Note

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

Matlab documentation of property attributes.

Definition at line 69 of file amimodel.m.

7.4.4.6 atol = 1e-8

Note

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

Matlab documentation of property attributes.

Default: 1e-8

Definition at line 79 of file amimodel.m.

7.4.4.7 rtol = 1e-8

Note

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

Matlab documentation of property attributes.

Default: 1e-8

Definition at line 90 of file amimodel.m.

7.4.4.8 maxsteps = 1e4

Note

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

Matlab documentation of property attributes.

Default: 1e4

Definition at line 101 of file amimodel.m.

7.4.4.9 debug = false

Note

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

Matlab documentation of property attributes.

Default: false

Definition at line 112 of file amimodel.m.

7.4.4.10 adjoint = true

Note

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

Matlab documentation of property attributes.

Default: true

Definition at line 124 of file amimodel.m.

7.4.4.11 forward = true

Note

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

Matlab documentation of property attributes.

Default: true

Definition at line 136 of file amimodel.m.

7.4.4.12 t0 = 0

Note

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

Matlab documentation of property attributes.

Default: 0

Definition at line 148 of file amimodel.m.

7.4.4.13 wtype

Note

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

Matlab documentation of property attributes.

Definition at line 159 of file amimodel.m.

7.4.4.14 nx

Note

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

Matlab documentation of property attributes.

Definition at line 169 of file amimodel.m.

7.4.4.15 nxtrue = 0

Note

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

Matlab documentation of property attributes.

Default: 0

Definition at line 179 of file amimodel.m.

7.4.4.16 ny

Note

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

Matlab documentation of property attributes.

Definition at line 190 of file amimodel.m.

7.4.4.17 nytrue = 0

Note

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

Matlab documentation of property attributes.

Default: 0

Definition at line 200 of file amimodel.m.

7.4.4.18 np

Note

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

Matlab documentation of property attributes.

Definition at line 211 of file amimodel.m.

7.4.4.19 nk

Note

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

Matlab documentation of property attributes.

Definition at line 221 of file amimodel.m.

7.4.4.20 nevent

Note

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

Matlab documentation of property attributes.

Definition at line 231 of file amimodel.m.

7.4.4.21 nz

Note

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

Matlab documentation of property attributes.

Definition at line 241 of file amimodel.m.

7.4.4.22 nztrue

Note

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

Matlab documentation of property attributes.

Definition at line 251 of file amimodel.m.

7.4.4.23 id

Note

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

Matlab documentation of property attributes.

Definition at line 261 of file amimodel.m.

7.4.4.24 ubw

Note

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

Matlab documentation of property attributes.

Definition at line 271 of file amimodel.m.

7.4.4.25 lbw

Note

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

Matlab documentation of property attributes.

Definition at line 281 of file amimodel.m.

7.4.4.26 nnz

Note

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

Matlab documentation of property attributes.

Definition at line 291 of file amimodel.m.

7.4.4.27 sparseidx

Note

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

Matlab documentation of property attributes.

Definition at line 301 of file amimodel.m.

7.4.4.28 rowvals

Note

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

Matlab documentation of property attributes.

Definition at line 311 of file amimodel.m.

7.4.4.29 colptrs

Note

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

Matlab documentation of property attributes.

Definition at line 321 of file amimodel.m.

7.4.4.30 sparseidxB

Note

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

Matlab documentation of property attributes.

Definition at line 331 of file amimodel.m.

7.4.4.31 rowvalsB

Note

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

Matlab documentation of property attributes.

Definition at line 341 of file amimodel.m.

7.4.4.32 colptrsB

Note

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

Matlab documentation of property attributes.

Definition at line 351 of file amimodel.m.

7.4.4.33 funs

Note

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

Matlab documentation of property attributes.

Definition at line 361 of file amimodel.m.

7.4.4.34 coptim = "-O3"

Note

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

Matlab documentation of property attributes.

Default: "-O3"

Definition at line 371 of file amimodel.m.

7.4.4.35 param = "lin"

Note

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

Matlab documentation of property attributes.

Default: "lin"

Definition at line 382 of file amimodel.m.

7.4.4.36 wrap_path

Note

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

Matlab documentation of property attributes.

Definition at line 393 of file amimodel.m.

7.4.4.37 recompile = false

Note

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

Matlab documentation of property attributes.

Default: false

Definition at line 403 of file amimodel.m.

7.4.4.38 cfun = struct("[]")

Note

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

Matlab documentation of property attributes.

Default: struct("[]")

Definition at line 414 of file amimodel.m.

7.4.4.39 o2flag = 0

Note

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

Matlab documentation of property attributes.

Default: 0

Definition at line 426 of file amimodel.m.

7.4.4.40 compver = 6

Note

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

Matlab documentation of property attributes.

Default: 6

Definition at line 442 of file amimodel.m.

7.4.4.41 z2event = double("[]")

Default: double("[]")

Definition at line 457 of file amimodel.m.

7.4.4.42 splineflag = false

Default: false

Definition at line 465 of file amimodel.m.

7.4.4.43 minflag = false

Default: false

Definition at line 473 of file amimodel.m.

7.4.4.44 maxflag = false

Default: false

Definition at line 481 of file amimodel.m.

7.4.4.45 nw = 0

Default: 0

Definition at line 489 of file amimodel.m.

7.4.4.46 ndwdx = 0

Default: 0

Definition at line 498 of file amimodel.m.

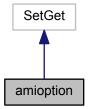
7.4.4.47 ndwdp = 0

Default: 0

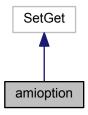
Definition at line 506 of file amimodel.m.

7.5 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

Public Attributes

• ::double atol = 1e-16

absolute integration tolerance

• ::double rtol = 1e-8

relative integration tolerance

• ::double maxsteps = 1e4 maximum number of steps for forward simulation • ::double sens_ind = double("[]") parameter index set for which sensitivies will be computed • ::double qpositivex = double("[]") state index set for which positivity will be enforced (EXPERIMENTAL FEATURE, USE WITH CARE) • ::double tstart = 0 timepoint at which the optimization starts • ::int Imm = 2 linear multistep method for forward problem • ::int iter = 2 iteration method for linear multistep for forward problem • ::int linsol = 9 linear solver • ::int stldet = true flag to activate stability limit detection • ::int interpType = 1 type of interpolation of forward solution in adjoint problem • ::int ImmB = 2 linear multistep method for adjoint problem • ::int iterB = 2 iteration method for linear multistep for adjoint problem • ::int ism = 1 method for forward sensitivity computation, this will only have an effect if forward sensitivities are requested • ::int sensi meth = 1 sensitivity method • ::int sensi = 0 number of orders for which sensitivities are requested, this will only have an effect if the appropriate code was compiled • ::int nmaxevent = 10 number of expected event occurences per event type • ::int ss = 0 flag indicating whether steady state sensitivites should be computed matlabtypesubstitute ordering = 1 pre-ordering scheme for the LU decomposition, this only applies if the sparse direct linear solver is used ::double sx0 = double("[]")

user provided initialization of sensitivity initial conditions

matlabtypesubstitute z2event = double("[]")

mapping of event outputs to events

matlabtypesubstitute id = double("[]")

index set of states with algebraic constraints

7.5.1 Detailed Description

Definition at line 17 of file amioption.m.

7.5.2 Constructor & Destructor Documentation

7.5.2.1 amioption (matlabtypesubstitute varargin)

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

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

OPTS = amioption(OLDOPTS, PARAM, VAL, ...) creates a copy of OLDOPTS with the named parameters altered with the specified value. OLDOPTS must not be of type amioption but can be a struct with the same fields

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

Parameters

varargin specification of non-default fields

Definition at line 222 of file amioption.m.

7.5.3 Member Data Documentation

7.5.3.1 atol = 1e-16

Default: 1e-16

Definition at line 28 of file amioption.m.

7.5.3.2 rtol = 1e-8

Default: 1e-8

Definition at line 36 of file amioption.m.

7.5.3.3 maxsteps = 1e4

Default: 1e4

Definition at line 44 of file amioption.m.

7.5.3.4 sens_ind = double("[]")

Default: double("[]")

Definition at line 52 of file amioption.m.

7.5.3.5 qpositivex = double("[]")

Default: double("[]")

Definition at line 60 of file amioption.m.

7.5.3.6 tstart = 0

Default: 0

Definition at line 68 of file amioption.m.

7.5.3.7 Imm = 2

Default: 2

Definition at line 76 of file amioption.m.

7.5.3.8 iter = 2

Default: 2

Definition at line 84 of file amioption.m.

7.5.3.9 linsol = 9

Default: 9

Definition at line 93 of file amioption.m.

7.5.3.10 stldet = true

Default: true

Definition at line 101 of file amioption.m.

7.5.3.11 interpType = 1

Default: 1

Definition at line 109 of file amioption.m.

7.5.3.12 ImmB = 2

Default: 2

Definition at line 117 of file amioption.m.

7.5.3.13 iterB = 2

Default: 2

Definition at line 125 of file amioption.m.

7.5.3.14 ism = 1

Default: 1

Definition at line 134 of file amioption.m.

7.5.3.15 sensi_meth = 1

Default: 1

Note

This property has custom functionality when its value is changed.

Definition at line 143 of file amioption.m.

```
7.5.3.16 sensi = 0
```

Default: 0

Note

This property has custom functionality when its value is changed.

Definition at line 151 of file amioption.m.

```
7.5.3.17 nmaxevent = 10
```

Default: 10

Definition at line 160 of file amioption.m.

```
7.5.3.18 ss = 0
```

Default: 0

Definition at line 168 of file amioption.m.

```
7.5.3.19 ordering = 1
```

Default: 1

Definition at line 176 of file amioption.m.

```
7.5.3.20 sx0 = double("[]")
```

Default: double("[]")

Definition at line 185 of file amioption.m.

```
7.5.3.21 z2event = double("[]")
```

Note

This property has the MATLAB attribute Hidden set to true.

```
Matlab documentation of property attributes.
```

```
Default: double("[]")
```

Definition at line 197 of file amioption.m.

```
7.5.3.22 id = double("[]")
```

Note

This property has the MATLAB attribute Hidden set to true.

```
Matlab documentation of property attributes.
```

Default: double("[]")

Definition at line 208 of file amioption.m.

7.6 ExpData Struct Reference

struct that carries all information about experimental data

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

Public Attributes

- double * am my
- double * am_ysigma
- double * am_mz
- double * am_zsigma

7.6.1 Detailed Description

Definition at line 18 of file edata.h.

7.6.2 Member Data Documentation

7.6.2.1 double * am_my

observed data

Definition at line 20 of file edata.h.

7.6.2.2 double* am_ysigma

standard deviation of observed data

Definition at line 22 of file edata.h.

7.6.2.3 double * am_mz

observed events

Definition at line 25 of file edata.h.

7.6.2.4 double* am_zsigma

standard deviation of observed events

Definition at line 27 of file edata.h.

7.7 funTest Class Reference

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

7.7.1 Detailed Description

Definition at line 17 of file funTest.m.

7.8 modelTest Class Reference

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

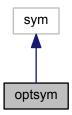
7.8.1 Detailed Description

Definition at line 17 of file modelTest.m.

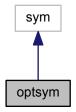
7.9 optsym Class Reference

OPTSYM is a placeholder class to get access to the protected sym.s.

Inheritance diagram for optsym:



Collaboration diagram for optsym:



Public Member Functions

- optsym (::sym symbol)
 optsym creates an optsym object from the symbolic expression symbol
- mlhsInnerSubst< matlabtypesubstitute > getoptimized ()
 getoptimized generates an optimized formulation of the expression of the symbolic expression obj. this optimized
 formulation identifies frequently employed expressions and subsitutes them by placeholder variables to avoid repeated
 evaluation

7.9.1 Detailed Description

Definition at line 17 of file optsym.m.

7.9.2 Constructor & Destructor Documentation

7.9.2.1 optsym (::sym symbol)

Parameters

symbol	symbolic expression
--------	---------------------

Definition at line 30 of file optsym.m.

7.9.3 Member Function Documentation

7.9.3.1 mlhsInnerSubst< matlabtypesubstitute > getoptimized ()

Return values

```
out optimized expression
```

Definition at line 41 of file optsym.m.

7.10 ReturnData Struct Reference

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

```
#include <rdata.h>
```

Public Attributes

- double * am tsdata
- double * am xdotdata
- double * am_dxdotdpdata
- double * am_dydxdata
- double * am_dydpdata
- double * am Jdata
- double * am_zdata
- double * am_zSdata
- double * am_xdata
- double * am_xSdata
- double * am ydata
- double * am_ySdata
- double * am_numstepsdata
- double * am_numstepsSdata
- double * am_numrhsevalsdata
- double * am_numrhsevalsSdata
- double * am_orderdata
- double * am_llhdata
- double * am chi2data
- double * am_IlhSdata
- double * am_llhS2data

7.10.1 Detailed Description

Definition at line 38 of file rdata.h.

7.10.2 Member Data Documentation

7.10.2.1 double* am_tsdata

timepoints

Definition at line 41 of file rdata.h.

7.10.2.2 double* am_xdotdata

time derivative

Definition at line 43 of file rdata.h.

7.10.2.3 double* am_dxdotdpdata

parameter derivative of time derivative

Definition at line 45 of file rdata.h.

7.10.2.4 double* am_dydxdata

state derivative of observables

Definition at line 47 of file rdata.h.

7.10.2.5 double* am_dydpdata

parameter derivative of observables

Definition at line 49 of file rdata.h.

7.10.2.6 double* am_Jdata

Jacobian of differential equation right hand side

Definition at line 51 of file rdata.h.

7.10.2.7 double* am_zdata

event output

Definition at line 53 of file rdata.h.

7.10.2.8 double* am_zSdata

parameter derivative of event output

Definition at line 55 of file rdata.h.

7.10.2.9 double * am_xdata

state

Definition at line 57 of file rdata.h.

7.10.2.10 double * am_xSdata

parameter derivative of state

Definition at line 59 of file rdata.h.

7.10.2.11 double* am_ydata

observable

Definition at line 61 of file rdata.h.

7.10.2.12 double* am_ySdata

parameter derivative of observable

Definition at line 63 of file rdata.h.

7.10.2.13 double * am_numstepsdata

number of integration steps forward problem

Definition at line 66 of file rdata.h.

7.10.2.14 double* am_numstepsSdata

number of integration steps backward problem

Definition at line 68 of file rdata.h.

7.10.2.15 double * am_numrhsevalsdata

number of right hand side evaluations forward problem

Definition at line 70 of file rdata.h.

7.10.2.16 double * am_numrhsevalsSdata

number of right hand side evaluations backwad problem

Definition at line 72 of file rdata.h.

7.10.2.17 double * am_orderdata

employed order forward problem

Definition at line 74 of file rdata.h.

7.10.2.18 double * am_llhdata

likelihood value

Definition at line 77 of file rdata.h.

7.10.2.19 double * am_chi2data

chi2 value

Definition at line 79 of file rdata.h.

7.10.2.20 double * am_IIhSdata

parameter derivative of likelihood

Definition at line 81 of file rdata.h.

7.10.2.21 double * am_llhS2data

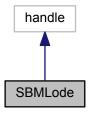
second order parameter derivative of likelihood

Definition at line 83 of file rdata.h.

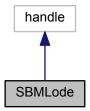
7.11 SBMLode Class Reference

SBMLODE carries all information about the differential equation defined by a SBML model definition file. This class acts as an interface between SBML files and amimodel.

Inheritance diagram for SBMLode:



Collaboration diagram for SBMLode:



Public Member Functions

• SBMLode (::char filename)

constructor of the SBMLode class. This takes the name of an SBML definition file and constructs an SBMLode object based on the parsed model

- noret::substitute importSBML (matlabtypesubstitute filename)
 - importSBML parses the SBML document and initialises the respective SBMLode object accordingly
- noret::substitute writeAMICI (matlabtypesubstitute modelname)

importSBML writes the information stored in the SBMLode object into an AMICI model definition file

Public Attributes

- ::symbolic state = sym("[]")
 - vector of non-constant and non-boundary states
- ::symbolic observable = sym("[]")
 - vector of guessed observables
- ::symbolic observable_name = sym("[]")

vector of guessed observable names

- ::symbolic param = sym("[]")
 - vector of SBML parameters

```
• ::symbolic parameter = sym("[]")
          vector of amimodel parameters
    • ::symbolic constant = sym("[]")
          vector of constant states
    ::symbolic compartment = sym("[]")
          vector of compartments
    ::symbolic volume = sym("[]")
          vector of compartment volumes
    ::symbolic initState = sym("[]")
          vector of initial values for non-constant and non-boundary states
    ::symbolic condition = sym("[]")
          vector of boundary condition states which are not constant
    • ::symbolic flux = sym("[]")
          vector of reaction fluxes
    ::symbolic stochiometry = sym("[]")
          matrix of reaction stochiometries
    • ::symbolic xdot = sym("[]")
          right hand side of differential equation for states
    ::symbolic trigger = sym("[]")
          vector of trigger functions for events
    ::symbolic bolus = sym("[]")
          matrix of event bolus
    • ::cell funmath = {""}
          cell array containing the function definition
    ::cell funarg = {""}
          cell array containing the function arguments
    ::char time_symbol = char("[]")
          expression for time in the model
    • ::sym pnom = double("[]")
          nominal parameter value
    • ::sym knom = double("[]")
          nominal condition value
7.11.1 Detailed Description
Definition at line 17 of file SBMLode.m.
7.11.2 Constructor & Destructor Documentation
7.11.2.1 SBMLode (::char filename)
Parameters
          filename
                      SBML definition file
Definition at line 192 of file SBMLode.m.
```

7.11.3.1 noret::substitute importSBML (matlabtypesubstitute modelname)

7.11.3 Member Function Documentation

Parameters

modelname	name of the sbml model file, without extension

Return values

this	initialised SBMLode object object

Definition at line 18 of file importSBML.m.

Here is the call graph for this function:



7.11.3.2 noret::substitute writeAMICI (matlabtypesubstitute modelname)

Parameters

modelname	target name of the AMICI model definition file, _syms will be appended
l I	$\gamma = \gamma$

Return values

this initialised SBMLode object object

Definition at line 18 of file writeAMICI.m.

7.11.4 Member Data Documentation

7.11.4.1 state = sym("[]")

Default: sym("[]")

Definition at line 29 of file SBMLode.m.

7.11.4.2 observable = sym("[]")

Default: sym("[]")

Definition at line 37 of file SBMLode.m.

7.11.4.3 observable_name = sym("[]")

Default: sym("[]")

Definition at line 45 of file SBMLode.m.

7.11.4.4 param = sym("[]")

Default: sym("[]")

Definition at line 53 of file SBMLode.m.

7.11.4.5 parameter = sym("[]") Default: sym("[]") Definition at line 61 of file SBMLode.m. 7.11.4.6 constant = sym("[]") Default: sym("[]") Definition at line 69 of file SBMLode.m. 7.11.4.7 compartment = sym("[]") Default: sym("[]") Definition at line 77 of file SBMLode.m. 7.11.4.8 volume = sym("[]") Default: sym("[]") Definition at line 85 of file SBMLode.m. 7.11.4.9 initState = sym("[]") Default: sym("[]") Definition at line 93 of file SBMLode.m. 7.11.4.10 condition = sym("[]") Default: sym("[]") Definition at line 101 of file SBMLode.m. 7.11.4.11 flux = sym("[]") Default: sym("[]") Definition at line 109 of file SBMLode.m. 7.11.4.12 stochiometry = sym("[]") Default: sym("[]") Definition at line 117 of file SBMLode.m. 7.11.4.13 xdot = sym("[]")

Default: sym("[]")

Definition at line 125 of file SBMLode.m.

```
7.11.4.14 trigger = sym("[]")
Default: sym("[]")
Definition at line 133 of file SBMLode.m.
7.11.4.15 bolus = sym("[]")
Default: sym("[]")
Definition at line 141 of file SBMLode.m.
7.11.4.16 funmath = {""}
Default: {""}
Definition at line 149 of file SBMLode.m.
7.11.4.17 funarg = {""}
Default: {""}
Definition at line 157 of file SBMLode.m.
7.11.4.18 time_symbol = char("[]")
Default: char("[]")
Definition at line 165 of file SBMLode.m.
7.11.4.19 pnom = double("[]")
Default: double("[]")
Definition at line 173 of file SBMLode.m.
7.11.4.20 knom = double("[]")
Default: double("[]")
Definition at line 181 of file SBMLode.m.
7.12 TempData Struct Reference
struct that provides temporary storage for different variables
#include <tdata.h>
Public Attributes
```

- realtype am_t
- N_Vector am_x
- N_Vector am_x_old
- N_Vector * am_x_disc
- N_Vector * am_xdot_disc

- N_Vector * am_xdot_old_disc
- N_Vector am_dx
- N_Vector am_dx_old
- N Vector am xdot
- N_Vector am_xdot_old
- N_Vector am_xB
- N_Vector am_xB_old
- N Vector am dxB
- N_Vector am_xQB
- N_Vector am_xQB_old
- N_Vector * am_sx
- N_Vector * am_sdx
- N Vector am id
- DIsMat am_Jtmp
- realtype * am_llhS0
- realtype am_g
- realtype * am_dgdp
- realtype * am_dgdx
- · realtype am_r
- realtype * am_drdp
- realtype * am_drdx
- · realtype am rval
- realtype * am drvaldp
- realtype * am_drvaldx
- realtype * am_dzdx
- realtype * am_dzdp
- realtype * am_dydp
- realtype * am_dydx
- realtype * am_yS0
- realtype * am_sigma_y
- realtype * am_dsigma_ydp
- realtype * am_sigma_z
- realtype * am_dsigma_zdp
- realtype * am_x_tmp
- realtype * am_sx_tmp
- realtype * am_dx_tmp
- realtype * am_sdx_tmp
- realtype * am_xdot_tmp
- realtype * am_xB_tmp
- realtype * am_xQB_tmp
- realtype * am_dxB_tmp
- realtype * am_id_tmp
- int * am_rootsfound
- int * am_rootidx
- int * am_nroots
- double * am_rootvals
- realtype * am_deltax
- realtype * am_deltasx
- realtype * am_deltaxB
- realtype * am_deltaqB
- int am_which
- realtype * am_discs
- realtype * am_irdiscs

7.12.1 Detailed Description

Definition at line 78 of file tdata.h.

7.12.2 Member Data Documentation

7.12.2.1 realtype am_t

current time

Definition at line 80 of file tdata.h.

7.12.2.2 N_Vector am_x

state vector

Definition at line 84 of file tdata.h.

7.12.2.3 N_Vector am_x_old

old state vector

Definition at line 86 of file tdata.h.

7.12.2.4 N_Vector* am_x_disc

array of state vectors at discontinuities

Definition at line 88 of file tdata.h.

7.12.2.5 N_Vector* am_xdot_disc

array of differential state vectors at discontinuities

Definition at line 90 of file tdata.h.

7.12.2.6 N_Vector* am_xdot_old_disc

array of old differential state vectors at discontinuities

Definition at line 92 of file tdata.h.

7.12.2.7 N_Vector am_dx

differential state vector

Definition at line 94 of file tdata.h.

7.12.2.8 N_Vector am_dx_old

old differential state vector

Definition at line 96 of file tdata.h.

7.12.2.9 N_Vector am_xdot

time derivative state vector

Definition at line 98 of file tdata.h.

7.12.2.10 N_Vector am_xdot_old

old time derivative state vector

Definition at line 100 of file tdata.h.

7.12.2.11 N_Vector am_xB

adjoint state vector

Definition at line 102 of file tdata.h.

7.12.2.12 N_Vector am_xB_old

old adjoint state vector

Definition at line 104 of file tdata.h.

7.12.2.13 N_Vector am_dxB

differential adjoint state vector

Definition at line 106 of file tdata.h.

7.12.2.14 N_Vector am_xQB

quadrature state vector

Definition at line 108 of file tdata.h.

7.12.2.15 N_Vector am_xQB_old

old quadrature state vector

Definition at line 110 of file tdata.h.

7.12.2.16 N_Vector* am_sx

sensitivity state vector array

Definition at line 112 of file tdata.h.

differential sensitivity state vector array

Definition at line 114 of file tdata.h.

7.12.2.18 N_Vector am_id

index indicating DAE equations vector

Definition at line 116 of file tdata.h.

7.12.2.19 DIsMat am_Jtmp

Jacobian

Definition at line 118 of file tdata.h.

7.12.2.20 realtype* am_llhS0

parameter derivative of likelihood array

Definition at line 121 of file tdata.h.

7.12.2.21 realtype am_g

data likelihood

Definition at line 123 of file tdata.h.

7.12.2.22 realtype* am_dgdp

parameter derivative of data likelihood

Definition at line 125 of file tdata.h.

7.12.2.23 realtype* am_dgdx

state derivative of data likelihood

Definition at line 127 of file tdata.h.

7.12.2.24 realtype am_r

event likelihood

Definition at line 129 of file tdata.h.

7.12.2.25 realtype* am_drdp

parameter derivative of event likelihood

Definition at line 131 of file tdata.h.

7.12.2.26 realtype* am_drdx

state derivative of event likelihood

Definition at line 133 of file tdata.h.

7.12.2.27 realtype am_rval

root function likelihood

Definition at line 135 of file tdata.h.

7.12.2.28 realtype* am_drvaldp

parameter derivative of root function likelihood

Definition at line 137 of file tdata.h.

7.12.2.29 realtype* am_drvaldx

state derivative of root function likelihood

Definition at line 139 of file tdata.h.

7.12.2.30 realtype* am_dzdx

state derivative of event

Definition at line 141 of file tdata.h.

7.12.2.31 realtype* am_dzdp

parameter derivative of event

Definition at line 143 of file tdata.h.

7.12.2.32 realtype* am_dydp

parameter derivative of observable

Definition at line 145 of file tdata.h.

7.12.2.33 realtype* am_dydx

state derivative of observable

Definition at line 147 of file tdata.h.

7.12.2.34 realtype* am_yS0

initial sensitivity of observable

Definition at line 149 of file tdata.h.

7.12.2.35 realtype* am_sigma_y

data standard deviation

Definition at line 151 of file tdata.h.

7.12.2.36 realtype* am_dsigma_ydp

parameter derivative of data standard deviation

Definition at line 153 of file tdata.h.

7.12.2.37 realtype* am_sigma_z

event standard deviation

Definition at line 155 of file tdata.h.

7.12.2.38 realtype* am_dsigma_zdp

parameter derivative of event standard deviation

Definition at line 157 of file tdata.h.

7.12.2.39 realtype* am_x_tmp

state array

Definition at line 160 of file tdata.h.

7.12.2.40 realtype* am_sx_tmp

sensitivity state array

Definition at line 162 of file tdata.h.

7.12.2.41 realtype* am_dx_tmp

differential state array

Definition at line 164 of file tdata.h.

7.12.2.42 realtype* am_sdx_tmp

differential sensitivity state array

Definition at line 166 of file tdata.h.

7.12.2.43 realtype* am_xdot_tmp

time derivative state array

Definition at line 168 of file tdata.h.

7.12.2.44 realtype* am_xB_tmp

differential adjoint state array

Definition at line 170 of file tdata.h.

7.12.2.45 realtype* am_xQB_tmp

quadrature state array

Definition at line 172 of file tdata.h.

7.12.2.46 realtype* am_dxB_tmp

differential adjoint state array

Definition at line 174 of file tdata.h.

7.12.2.47 realtype* am_id_tmp

index indicating DAE equations array

Definition at line 176 of file tdata.h.

7.12.2.48 int* am_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, rootsfound[i]?= 0 if gi has a root, and = 0 if not.

Definition at line 183 of file tdata.h.

7.12.2.49 int* am rootidx

array of index which root has been found

Definition at line 185 of file tdata.h.

7.12.2.50 int* am_nroots

array of number of found roots for a certain event type

Definition at line 187 of file tdata.h.

7.12.2.51 double* am_rootvals

array of values of the root function

Definition at line 189 of file tdata.h.

7.12.2.52 realtype* am_deltax

change in x

Definition at line 193 of file tdata.h.

7.12.2.53 realtype* am_deltasx

change in sx

Definition at line 195 of file tdata.h.

7.12.2.54 realtype* am_deltaxB

change in xB

Definition at line 197 of file tdata.h.

7.12.2.55 realtype* am_deltaqB

change in qB

Definition at line 199 of file tdata.h.

7.12.2.56 int am_which

integer for indexing of backwards problems

Definition at line 203 of file tdata.h.

7.12.2.57 realtype* am_discs

array containing the time-points of discontinuities

Definition at line 206 of file tdata.h.

7.12.2.58 realtype* am_irdiscs

array containing the index of discontinuities

Definition at line 208 of file tdata.h.

7.13 UserData Struct Reference

struct that stores all user provided data

```
#include <udata.h>
```

Public Attributes

- double * am_qpositivex
- int * am_plist
- int am_np
- int am_ny
- int am_nytrue
- int am_nx
- int am_nz
- int am_nztrue
- int am_ne
- int am_nt
- int am_nw
- int am_ndwdx
- int am_ndwdp
- int am_nnz
- int am_nmaxevent
- double * am_p
- double * am k
- double am_tstart
- double * am_ts
- double * am_pbar
- double * am_xbar
- double * am idlist
- int am_sensi
- double am_atol
- double am_rtol

- int am_maxsteps
- int am_ism
- int am_sensi_meth
- int am_linsol
- int am_interpType
- int am_lmm
- int am_iter
- booleantype am_stldet
- int am_ubw
- int am_lbw
- booleantype am_bsx0
- double * am_sx0data
- int am_event_model
- int am_data_model
- int am_ordering
- double * am_z2event
- double * am_h
- SIsMat am_J
- realtype * am_dxdotdp
- realtype * am_w
- realtype * am_dwdx
- realtype * am_dwdp
- realtype * am_M
- realtype * am_dfdx
- booleantype am_nan_dxdotdp
- booleantype am_nan_J
- booleantype am_nan_JSparse
- booleantype am_nan_xdot
- booleantype am_nan_xBdot
- booleantype am_nan_qBdot

7.13.1 Detailed Description

Definition at line 78 of file udata.h.

7.13.2 Member Data Documentation

7.13.2.1 double* am_qpositivex

positivity flag

Definition at line 80 of file udata.h.

 $\textbf{7.13.2.2} \quad \textbf{int}* \ \textbf{am_plist}$

parameter reordering

Definition at line 83 of file udata.h.

7.13.2.3 int am_np

number of parameters

Definition at line 85 of file udata.h.

7.13.2.4 int am_ny

number of observables

Definition at line 87 of file udata.h.

7.13.2.5 int am_nytrue

number of observables in the unaugmented system

Definition at line 89 of file udata.h.

7.13.2.6 int am_nx

number of states

Definition at line 91 of file udata.h.

7.13.2.7 int am_nz

number of event outputs

Definition at line 93 of file udata.h.

7.13.2.8 int am_nztrue

number of event outputs in the unaugmented system

Definition at line 95 of file udata.h.

7.13.2.9 int am_ne

number of events

Definition at line 97 of file udata.h.

7.13.2.10 int am_nt

number of timepoints

Definition at line 99 of file udata.h.

7.13.2.11 int am_nw

number of common expressions

Definition at line 101 of file udata.h.

7.13.2.12 int am_ndwdx

number of derivatives of common expressions wrt x

Definition at line 103 of file udata.h.

7.13.2.13 int am_ndwdp

number of derivatives of common expressions wrt p

Definition at line 105 of file udata.h.

7.13.2.14 int am_nnz

number of nonzero entries in jacobian

Definition at line 107 of file udata.h.

7.13.2.15 int am_nmaxevent

maximal number of events to track

Definition at line 109 of file udata.h.

7.13.2.16 double * am_p

parameter array

Definition at line 112 of file udata.h.

7.13.2.17 double* am_k

constants array

Definition at line 114 of file udata.h.

7.13.2.18 double am_tstart

starting time

Definition at line 117 of file udata.h.

7.13.2.19 double* am_ts

timepoints

Definition at line 119 of file udata.h.

7.13.2.20 double * am_pbar

scaling of parameters

Definition at line 122 of file udata.h.

7.13.2.21 double * am_xbar

scaling of states

Definition at line 124 of file udata.h.

7.13.2.22 double* am_idlist

flag array for DAE equations

Definition at line 127 of file udata.h.

7.13.2.23 int am_sensi

flag indicating whether sensitivities are supposed to be computed

Definition at line 130 of file udata.h.

7.13.2.24 double am_atol

absolute tolerances for integration

Definition at line 132 of file udata.h.

7.13.2.25 double am_rtol

relative tolerances for integration

Definition at line 134 of file udata.h.

7.13.2.26 int am_maxsteps

maximum number of allowed integration steps

Definition at line 136 of file udata.h.

7.13.2.27 int am_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 142 of file udata.h.

7.13.2.28 int am_sensi_meth

method for sensitivity computation

CW FSA for forward sensitivity analysis, CW ASA for adjoint sensitivity analysis

Definition at line 148 of file udata.h.

7.13.2.29 int am_linsol

linear solver specification

Definition at line 150 of file udata.h.

7.13.2.30 int am_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 155 of file udata.h.

7.13.2.31 int am_lmm

linear multistep method

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

Definition at line 161 of file udata.h.

7.13.2.32 int am_iter

nonlinear solver

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

Definition at line 167 of file udata.h.

7.13.2.33 booleantype am_stldet

flag controlling stability limit detection

Definition at line 170 of file udata.h.

7.13.2.34 int am_ubw

upper bandwith of the jacobian

Definition at line 173 of file udata.h.

7.13.2.35 int am_lbw

lower bandwith of the jacobian

Definition at line 175 of file udata.h.

7.13.2.36 booleantype am_bsx0

flag for sensitivity initialisation

flag which determines whether analytic sensitivities initialisation or provided initialisation should be used

Definition at line 181 of file udata.h.

7.13.2.37 double * am_sx0data

sensitivity initialisation

Definition at line 184 of file udata.h.

7.13.2.38 int am_event_model

error model for events

Definition at line 187 of file udata.h.

7.13.2.39 int am_data_model

error model for udata

Definition at line 189 of file udata.h.

7.13.2.40 int am_ordering

state ordering

Definition at line 192 of file udata.h.

7.13.2.41 double* am z2event

index indicating to which event an event output belongs

Definition at line 195 of file udata.h.

7.13.2.42 double * am h

flag indicating whether a certain heaviside function should be active or not

Definition at line 198 of file udata.h.

7.13.2.43 SIsMat am_J

tempory storage of Jacobian data across functions

Definition at line 201 of file udata.h.

7.13.2.44 realtype* am_dxdotdp

tempory storage of dxdotdp data across functions

Definition at line 203 of file udata.h.

7.13.2.45 realtype* am_w

tempory storage of w data across functions

Definition at line 205 of file udata.h.

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7.13.2.46 realtype* am_dwdx

tempory storage of dwdx data across functions

Definition at line 207 of file udata.h.

7.13.2.47 realtype* am_dwdp

tempory storage of dwdp data across functions

Definition at line 209 of file udata.h.

7.13.2.48 realtype* am_M

tempory storage of M data across functions

Definition at line 211 of file udata.h.

7.13.2.49 realtype* am_dfdx

tempory storage of dfdx data across functions

Definition at line 213 of file udata.h.

7.13.2.50 booleantype am_nan_dxdotdp

flag indicating whether a NaN in dxdotdp has been reported

Definition at line 216 of file udata.h.

7.13.2.51 booleantype am_nan_J

flag indicating whether a NaN in J has been reported

Definition at line 218 of file udata.h.

7.13.2.52 booleantype am_nan_JSparse

flag indicating whether a NaN in JSparse has been reported

Definition at line 220 of file udata.h.

7.13.2.53 booleantype am_nan_xdot

flag indicating whether a NaN in xdot has been reported

Definition at line 222 of file udata.h.

7.13.2.54 booleantype am_nan_xBdot

flag indicating whether a NaN in xBdot has been reported

Definition at line 224 of file udata.h.

7.13.2.55 booleantype am_nan_qBdot

flag indicating whether a NaN in qBdot has been reported

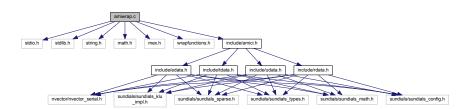
Definition at line 226 of file udata.h.

8 File Documentation

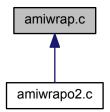
8.1 amiwrap.c File Reference

core routines for mex interface

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <math.h>
#include <mex.h>
#include "wrapfunctions.h"
#include <include/amici.h>
Include dependency graph for amiwrap.c:
```



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



Macros

- #define USE MATH DEFINES
- #define M_PI 3.14159265358979323846

Functions

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

8.1.1 Detailed Description

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

8.1.2 Macro Definition Documentation

8.1.2.1 #define _USE_MATH_DEFINES

MS definition of PI and other constants

Definition at line 12 of file amiwrap.c.

8.1.2.2 #define M_PI 3.14159265358979323846

numeric definition of PI for settings where the system does not provide one

Definition at line 16 of file amiwrap.c.

8.1.3 Function Documentation

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

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

Parameters

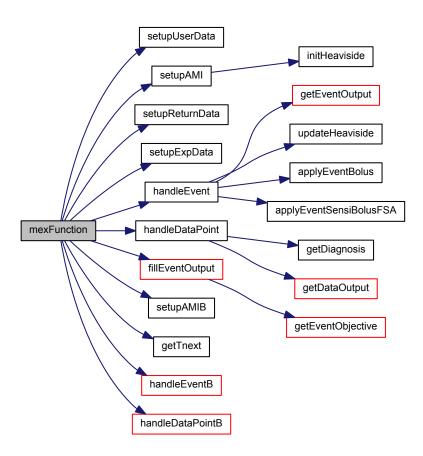
in	nlhs	number of output arguments of the matlab call		
		Type: int		
out	plhs	ointer to the array of output arguments		
		Type: mxArray		
in	nrhs	number of input arguments of the matlab call		
		Type: int		
in	prhs	pointer to the array of input arguments		
		Type: mxArray		

Returns

void

Definition at line 31 of file amiwrap.c.

Here is the call graph for this function:



8.2 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.

8.2.1 Function Documentation

8.2.1.1 noret::substitute amiwrap (matlabtypesubstitute varargin)

Parameters

varargin

1 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 simualation file
- symfun specifies a function which executes model defition see Model Definition for details
- tdir target directory where the simulation file should be placed **Default:** \$AMI-CIDIR/models/modelname
- o2flag boolean whether second order sensitivities should be enabled **Default**: false

Return values

-04	المامان
021180	VOID

Definition at line 17 of file amiwrap.m.

8.3 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.

8.3.1 Function Documentation

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

Parameters

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

Return values

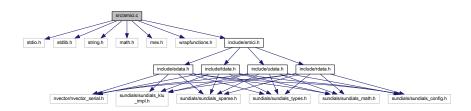
modelname	void

Definition at line 17 of file SBML2AMICI.m.

8.4 src/amici.c File Reference

core routines for integration

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <math.h>
#include <mex.h>
#include "wrapfunctions.h"
#include <include/amici.h>
Include dependency graph for amici.c:
```



Macros

- #define USE MATH DEFINES
- #define M_PI 3.14159265358979323846
- #define initField2(FIELD, D1, D2)

initField2 initialises an field of mxsol with an empty matrix and attaches FIELDdata as data pointer

#define initField3(FIELD, D1, D2, D3)

initField3 initialises an field of mxsol with an empty tensor and attaches FIELDdata as data pointer

• #define readOptionScalar(OPTION, TYPE)

readOptionScalar reads the scalar property from the options struct and casts it to the specified type

#define readOptionData(OPTION)

readOptionData reads the matrix property from the options struct

#define AMI_SUCCESS 0

Functions

- UserData setupUserData (const mxArray *prhs[])
- ReturnData setupReturnData (mxArray *plhs[], void *user_data, double *pstatus)
- ExpData setupExpData (const mxArray *prhs[], void *user_data)
- void * setupAMI (int *status, void *user_data, void *temp_data)
- void setupAMIB (int *status, void *ami_mem, void *user_data, void *temp_data)
- void getDataSensisFSA (int *status, int it, void *ami_mem, void *user_data, void *return_data, void *exp_data, void *temp_data)
- void getDataSensisASA (int *status, int it, void *ami_mem, void *user_data, void *return_data, void *exp data, void *temp data)
- void getDataOutput (int *status, int it, void *ami_mem, void *user_data, void *return_data, void *exp_data, void *temp data)
- void getEventSensisFSA (int *status, int ie, void *ami_mem, void *user_data, void *return_data, void *temp_data)
- void getEventSensisFSA_tf (int *status, int ie, void *ami_mem, void *user_data, void *return_data, void *temp data)
- void getEventSensisASA (int *status, int ie, void *ami_mem, void *user_data, void *return_data, void *exp_data, void *temp_data)
- void getEventSigma (int *status, int ie, int iz, void *ami_mem, void *user_data, void *return_data, void *exp_data, void *temp_data)

- void getEventObjective (int *status, int ie, void *ami_mem, void *user_data, void *return_data, void *exp_data, void *temp_data)
- void getEventOutput (int *status, realtype *tlastroot, void *ami_mem, void *user_data, void *return_data, void *exp_data, void *temp_data)
- void fillEventOutput (int *status, void *ami_mem, void *user_data, void *return_data, void *exp_data, void *temp_data)
- void handleDataPoint (int *status, int it, void *ami_mem, void *user_data, void *return_data, void *exp_data, void *temp_data)
- void handleDataPointB (int *status, int it, void *ami_mem, void *user_data, void *return_data, void *temp data)
- void handleEvent (int *status, int iroot, realtype *tlastroot, void *ami_mem, void *user_data, void *return_data, void *exp_data, void *temp_data)
- void handleEventB (int *status, int iroot, void *ami_mem, void *user_data, void *temp_data)
- realtype getTnext (realtype *troot, int iroot, realtype *tdata, int it, void *user_data)
- void applyEventBolus (int *status, void *ami_mem, void *user_data, void *temp_data)
- void applyEventSensiBolusFSA (int *status, void *ami_mem, void *user_data, void *temp_data)
- void initHeaviside (int *status, void *user_data, void *temp_data)
- void updateHeaviside (int *status, void *user_data, void *temp_data)
- void updateHeavisideB (int *status, int iroot, void *user data, void *temp data)
- void getDiagnosis (int *status, int it, void *ami_mem, void *user_data, void *return_data)
- void getDiagnosisB (int *status, int it, void *ami_mem, void *user_data, void *return_data, void *temp_data)

8.4.1 Macro Definition Documentation

8.4.1.1 #define _USE_MATH_DEFINES

return value indicating successful execution MS definition of PI and other constants

Definition at line 12 of file amici.c.

8.4.1.2 #define M_PI 3.14159265358979323846

numeric definition of PI for settings where the system does not provide one

Definition at line 16 of file amici.c.

8.4.1.3 #define initField2(FIELD, D1, D2)

Value:

```
mxArray *mx ## FIELD; \
mx ## FIELD = mxCreateDoubleMatrix(D1,D2,mxREAL); \
FIELD ## data = mxGetPr(mx ## FIELD); \
mxSetField(mxsol,0,#FIELD,mx ## FIELD)
```

Parameters

in	FIELD	name of the field
		Type: char
in	D1	number of rows
		Type: int
in	D2	number of columns
		Type: int

Definition at line 28 of file amici.c.

8.4.1.4 #define initField3(FIELD, D1, D2, D3)

Value:

```
mxArray *mx ## FIELD; \
const mwSize dims ## FIELD[]={D1,D2,D3}; \
mx ## FIELD = mxCreateNumericArray(3,dims ## FIELD,mxDOUBLE_CLASS,mxREAL); \
FIELD ## data = mxGetPr(mx ## FIELD); \
mxSetField(mxsol,0,#FIELD,mx ## FIELD)
```

Parameters

in	FIELD	name of the field
		Type: char
in	D1	number of rows
		Type: int
in	D2	number of columns
		Type: int
in	D3	size of third dimension
		Type: int

Definition at line 41 of file amici.c.

8.4.1.5 #define readOptionScalar(OPTION, TYPE)

Value:

```
if (mxGetProperty(prhs[3],0,#OPTION)) {
    OPTION = (TYPE)mxGetScalar(mxGetProperty(prhs[3],0,#OPTION)); \
} else { \
    mexWarnMsgIdAndTxt("AMICI:mex:OPTION","Provided options are not of class amioption!"); \
    return(NULL); \
}
```

Parameters

in	OPTION	name of the field
		Type: char
in	TYPE	number of rows
		Type: type

Definition at line 53 of file amici.c.

8.4.1.6 #define readOptionData(OPTION)

Value:

```
if (mxGetProperty(prhs[3],0,#OPTION)) {
    OPTION = mxGetData(mxGetProperty(prhs[3],0,#OPTION)); \
} else { \
    mexWarnMsgIdAndTxt("AMICI:mex:OPTION","Provided options are not of class amioption!"); \
    return(NULL); \
}
```

Parameters

in	OPTION	name of the field
		Type: char

Definition at line 65 of file amici.c.

8.4.1.7 #define AMI_SUCCESS 0

definition of the return value for successful function evaluations

Definition at line 74 of file amici.c.

8.4.2 Function Documentation

2/21	HearData	setupUserData (conet my Array	+ nrhc[1 \
0.4.2.1	userbala	setubuserbata t	CONST IIIXAMAN	* DITISL L

setupUserData extracts information from the matlab call and returns the corresponding UserData struct

Parameters

in	prhs	pointer to the array of input arguments
		Type: mxArray

Returns

udata: struct containing all provided user data

Type: UserData

Definition at line 76 of file amici.c.

Here is the caller graph for this function:



8.4.2.2 ReturnData setupReturnData (mxArray * plhs[], void * user_data, double * pstatus)

setupReturnData initialises the return data struct

Parameters

in	plhs	user input
		Type: *mxArray
in	user_data	pointer to the user data struct
		Type: UserData
in	pstatus	pointer to the current status flag
		Type: *double

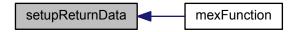
Returns

rdata: return data struct **Type**: ReturnData

user udata

Definition at line 220 of file amici.c.

Here is the caller graph for this function:



8.4.2.3 ExpData setupExpData (const mxArray * prhs[], void * user_data)

setupExpData initialises the experimental data struct

Parameters

in	prhs	user input
		Type: *mxArray
in	user_data	pointer to the user data struct
		Type: UserData

Returns

edata: experimental data struct

Type: ExpData

user udata

Definition at line 304 of file amici.c.

Here is the caller graph for this function:



8.4.2.4 void* setupAMI (int * status, void * user_data, void * temp_data)

setupAMIs initialises the ami memory object

Parameters

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

Returns

ami_mem pointer to the cvodes/idas memory block

Definition at line 406 of file amici.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.2.5 void setupAMIB (int * status, void * ami_mem, void * user_data, void * temp_data)

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	user_data	pointer to the user data struct
		Type: UserData
in	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

ami_mem pointer to the cvodes/idas memory block for the backward problem

Definition at line 725 of file amici.c.

Here is the caller graph for this function:



8.4.2.6 void getDataSensisFSA (int * status, int it, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

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	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 920 of file amici.c.

Here is the caller graph for this function:



8.4.2.7 void getDataSensisASA (int * status, int it, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

getDataSensisASA extracts data information for adjoint sensitivity analysis

Parameters

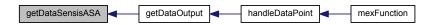
t-	-t-t	flow indication accesses of acceptains
out	status	flag indicating success of execution
		Type: *int
in	it	index of current timepoint
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 968 of file amici.c.

Here is the caller graph for this function:



8.4.2.8 void getDataOutput (int * status, int it, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

getDataOutput extracts output information for data-points

Parameters

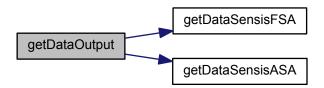
out	status	flag indicating success of execution
		Type: ∗int
in	it	index of current timepoint
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1016 of file amici.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.2.9 void getEventSensisFSA (int * status, int ie, void * ami_mem, void * user_data, void * return_data, void * temp_data)

getEventSensisFSA extracts event information for forward sensitivity analysis

Parameters

out	status	flag indicating success of execution
		Type: int
in	ie	index of event type
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1068 of file amici.c.

Here is the caller graph for this function:



8.4.2.10 void getEventSensisFSA_tf (int * status, int ie, void * ami_mem, void * user_data, void * return_data, void * temp_data)

getEventSensisFSA_tf extracts event information for forward sensitivity analysis for events that happen at the end of the considered interval

Parameters

out	status	flag indicating success of execution
		Type: int
in	ie	index of event type
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1098 of file amici.c.

Here is the caller graph for this function:



8.4.2.11 void getEventSensisASA (int * status, int ie, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

getEventSensisASA extracts event information for adjoint sensitivity analysis

Parameters

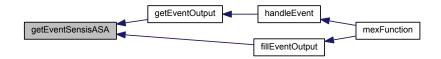
out	status	flag indicating success of execution
		Type: *int
in	ie	index of event type
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1129 of file amici.c.

Here is the caller graph for this function:



8.4.2.12 void getEventSigma (int * status, int ie, int iz, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

getEventSigma extracts fills sigma_z either from the user defined function or from user input

Parameters

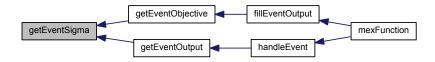
out	status	flag indicating success of execution
		Type: *int
in	ie	event type index
		Type: int
in	iz	event output index
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1193 of file amici.c.

Here is the caller graph for this function:



8.4.2.13 void getEventObjective (int * status, int ie, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

getEventObjective updates the objective function on the occurence of an event

Parameters

out	status	flag indicating success of execution
		Type: *int
in	ie	event type index
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1230 of file amici.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.2.14 void getEventOutput (int * status, realtype * tlastroot, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

getEventOutput extracts output information for events

Parameters

out	status	flag indicating success of execution
		Type: *int

in	tlastroot	timepoint of last occured event
		Type: *realtype
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

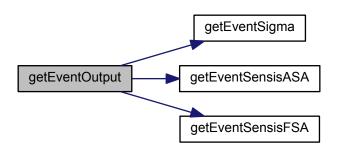
Returns

cv_status updated status flag

Type: int

Definition at line 1274 of file amici.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.2.15 void fillEventOutput (int * status, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

fillEventOutput fills missing roots at last timepoint

Parameters

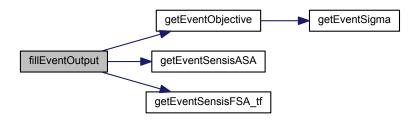
out	status	flag indicating success of execution
		Type: *int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1341 of file amici.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.2.16 void handleDataPoint (int * status, int it, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

handleDataPoint executes everything necessary for the handling of data points

Parameters

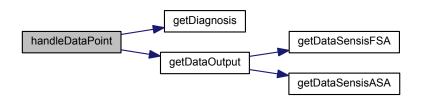
out	status	flag indicating success of execution
		Type: *int
in	it	index of data point
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1393 of file amici.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.2.17 void handleDataPointB (int * status, int it, void * ami_mem, void * user_data, void * return_data, void * temp_data)

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

Parameters

out	status	flag indicating success of execution
		Type: *int
in	it	index of data point
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1458 of file amici.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.2.18 void handleEvent (int * status, int iroot, realtype * tlastroot, void * ami_mem, void * user_data, void * return_data, void * exp_data, void * temp_data)

handleEvent executes everything necessary for the handling of events

out	status	flag indicating success of execution
		Type: *int

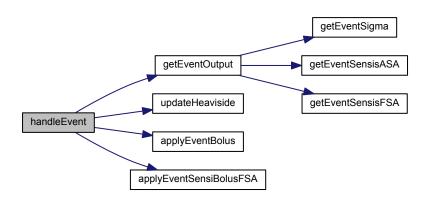
out	iroot	index of event
		Type: int
out	tlastroot	pointer to the timepoint of the last event
		Type: ∗realtype
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
in	exp_data	pointer to the experimental data struct
		Type: ExpData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1489 of file amici.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.2.19 void handleEventB (int * status, int iroot, void * ami_mem, void * user_data, void * temp_data)

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

Parameters

out	status	flag indicating success of execution
		Type: *int
out	iroot	index of event
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

cv_status updated status flag

Type: int

Definition at line 1590 of file amici.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.4.2.20 realtype getTnext (realtype * troot, int iroot, realtype * tdata, int it, void * user_data)

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

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	user_data	pointer to the user data struct
		Type: UserData

Returns

tnext next timepoint **Type**: realtype

Definition at line 1648 of file amici.c.

Here is the caller graph for this function:



8.4.2.21 void applyEventBolus (int * status, void * ami_mem, void * user_data, void * temp_data)

applyEventBolus applies the event bolus to the current state

Parameters

out	status	flag indicating success of execution
		Type: *int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1693 of file amici.c.

Here is the caller graph for this function:



8.4.2.22 void applyEventSensiBolusFSA (int * status, void * ami_mem, void * user_data, void * temp_data)

applyEventSensiBolusFSA applies the event bolus to the current sensitivities

Parameters

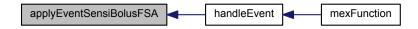
out	status	flag indicating success of execution
		Type: *int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1728 of file amici.c.

Here is the caller graph for this function:



8.4.2.23 void initHeaviside (int * status, void * user_data, void * temp_data)

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

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

Returns

void

Definition at line 1766 of file amici.c.

Here is the caller graph for this function:



8.4.2.24 void updateHeaviside (int * status, void * user_data, void * temp_data)

updateHeaviside updates the heaviside variables h on event occurences

Parameters

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

Returns

void

Definition at line 1799 of file amici.c.

Here is the caller graph for this function:



8.4.2.25 void updateHeavisideB (int * status, int iroot, void * user_data, void * temp_data)

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

out	status	flag indicating success of execution
		Type: *int

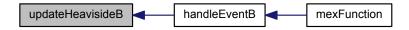
in	iroot	discontinuity occurance index
		Type: int
in	user_data	pointer to the user data struct
		Type: UserData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1828 of file amici.c.

Here is the caller graph for this function:



8.4.2.26 void getDiagnosis (int * status, int it, void * ami_mem, void * user_data, void * return_data)

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

out	status	flag indicating success of execution
		Type: *int
in	it	time-point index
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData

Returns

void

Definition at line 1858 of file amici.c.

Here is the caller graph for this function:



8.4.2.27 void getDiagnosisB (int * status, int it, void * ami_mem, void * user_data, void * return_data, void * temp_data) getDiagnosisB extracts diagnosis information from solver memory block and writes them into the return data struct for the backward problem

Parameters

out	status	flag indicating success of execution
		Type: *int
in	it	time-point index
		Type: int
in	ami_mem	pointer to the solver memory block
		Type: *void
in	user_data	pointer to the user data struct
		Type: UserData
out	return_data	pointer to the return data struct
		Type: ReturnData
out	temp_data	pointer to the temporary data struct
		Type: TempData

Returns

void

Definition at line 1896 of file amici.c.

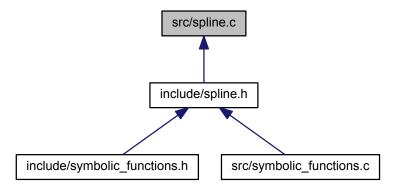
Here is the caller graph for this function:



8.5 src/spline.c File Reference

definition of spline functions

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



Functions

- static int spline (int n, int end1, int end2, double slope1, double slope2, double x[], double y[], double b[], double c[], double d[])
- static double seval (int n, double u, double x[], double y[], double b[], double c[], double d[])
- static double deriv (int n, double u, double x[], double b[], double c[], double d[])
- static double sinteg (int n, double u, double x[], double y[], double b[], double c[], double d[])

8.5.1 Detailed Description

Author

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

8.5.2 Function Documentation

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

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

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

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

Parameters

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

Return values

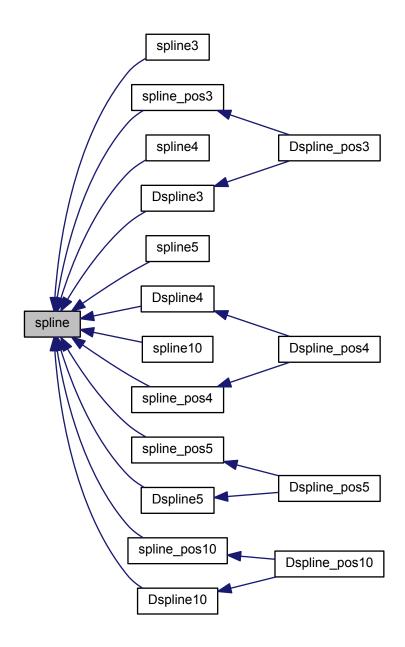
0	normal return
1	less than two data points; cannot interpolate
2	x[] are not in ascending order

Notes

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

Definition at line 66 of file spline.c.

Here is the caller graph for this function:



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

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

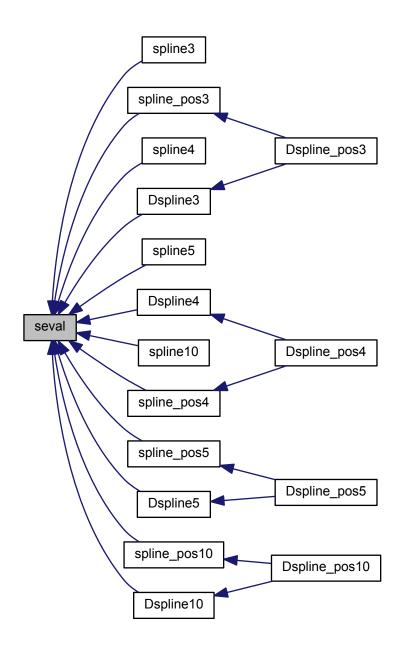
the value of the spline function at u

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.c.

Here is the caller graph for this function:



8.5.2.3 static double deriv (int n, double u, double x[], double b[], double c[], double d[]) [static]

Evaluate the derivative of the cubic spline function

S(x) = B[i] + 2.0 * C[i] * w + 3.0 * D[i] * w **2 where w = u - X[i] and X[i] <= u <= X[i+1] Note that Horner's rule is used. If <math>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 derivative is to be evaluated
in	X	the abscissas of the knots in strictly increasing order
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 derivative 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 264 of file spline.c.

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

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.

Parameters

in	n	the number of data points or knots ($n \ge 2$)
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.

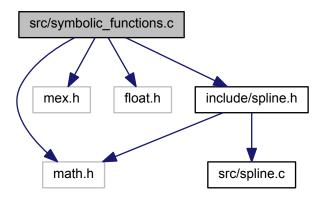
Definition at line 324 of file spline.c.

8.6 src/symbolic_functions.c File Reference

definition of symbolic functions

```
#include <math.h>
#include <mex.h>
#include <float.h>
#include <include/spline.h>
```

Include dependency graph for symbolic_functions.c:



Macros

- #define TRUE 1
- #define FALSE 0

Functions

- double amilog (double x)
- double heaviside (double x)
- double sign (double x)
- double am_min (double a, double b)
- double Dam_min (int id, double a, double b)
- double am max (double a, double b)
- double Dam max (int id, double a, double b)
- double spline3 (double t, double t1, double p1, double t2, double p2, double t3, double p3, int ss, double dudt)
- double spline_pos3 (double t, double t1, double p1, double t2, double p2, double t3, double p3, int ss, double dudt)
- double spline4 (double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, int ss, double dudt)
- double spline_pos4 (double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, int ss, double dudt)
- double spline5 (double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, double t5, double p5, int ss, double dudt)
- double spline_pos5 (double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, double t5, double p5, int ss, double dudt)
- double spline10 (double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, double t5, double p5, double t6, double p6, double t7, double p7, double t8, double p8, double t9, double p9, double t10, double p10, int ss, double dudt)
- double spline_pos10 (double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, double t5, double p5, double t6, double p6, double t7, double p7, double t8, double p8, double t9, double p9, double t10, double p10, int ss, double dudt)
- double Dspline3 (int id, double t, double t1, double p1, double t2, double p2, double t3, double p3, int ss, double dudt)

• double Dspline_pos3 (int id, double t, double t1, double p1, double t2, double p2, double t3, double p3, int ss, double dudt)

- double Dspline4 (int id, double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, int ss, double dudt)
- double Dspline_pos4 (int id, double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, int ss, double dudt)
- double Dspline5 (int id, double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, double t5, double p5, int ss, double dudt)
- double Dspline_pos5 (int id, double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, double t5, double p5, int ss, double dudt)
- double Dspline10 (int id, double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, double t5, double p5, double t6, double p6, double t7, double p7, double t8, double p8, double t9, double p9, double t10, double p10, int ss, double dudt)
- double Dspline_pos10 (int id, double t, double t1, double p1, double t2, double p2, double t3, double p3, double t4, double p4, double t5, double p5, double t6, double p6, double t7, double p7, double t8, double p8, double t9, double p10, int ss, double dudt)

8.6.1 Detailed Description

This file contains definitions of various symbolic functions which

8.6.2 Macro Definition Documentation

8.6.2.1 #define TRUE 1

bool return value true

Definition at line 16 of file symbolic functions.c.

8.6.2.2 #define FALSE 0

bool return value false

Definition at line 18 of file symbolic_functions.c.

8.6.3 Function Documentation

8.6.3.1 double amilog (double x)

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

Parameters

x argument

Returns

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

Definition at line 28 of file symbolic_functions.c.

8.6.3.2 double heaviside (double x)

c implementation of matlab function heaviside

Parameters

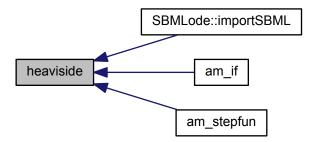
X	argument
---	----------

Returns

if(x>0) then 1 else 0

Definition at line 43 of file symbolic_functions.c.

Here is the caller graph for this function:



8.6.3.3 double sign (double x)

c implementation of matlab function sign

Parameters

X	argument

Returns

0

Type: double

Definition at line 58 of file symbolic_functions.c.

8.6.3.4 double am_min (double a, double b)

c implementation of matlab function min

Parameters

а	value1
	Type: double
b	value2
	Type: double

Returns

if(a < b) then a else b

Type: double

Definition at line 78 of file symbolic_functions.c.

8.6.3.5 double Dam_min (int id, double a, double b)

parameter derivative of c implementation of matlab function min

Parameters

id	argument index for differentiation
а	bool1
	Type: double
b	bool2
	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 92 of file symbolic_functions.c.

8.6.3.6 double am_max (double a, double b)

c implementation of matlab function max

Parameters

а	value1
	Type: double
b	value2
	Type: double

Returns

if(a > b) then a else b

Type: double

Definition at line 116 of file symbolic_functions.c.

8.6.3.7 double Dam_max (int id, double a, double b)

parameter derivative of c implementation of matlab function max

Parameters

id	argument index for differentiation
а	bool1
	Type: double
b	bool2
	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 130 of file symbolic_functions.c.

8.6.3.8 double spline3 (double t, doub

Parameters

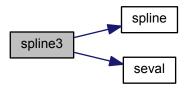
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 162 of file symbolic_functions.c.

Here is the call graph for this function:



8.6.3.9 double spline_pos3 (double t, double t1, double t2, double t2, double t3, double t3, double t3, int t5, double t4 positive spline function with 3 nodes

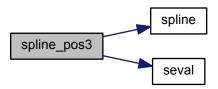
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 203 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.6.3.10 double spline4 (double t, double t, double p, double t, dou

spline function with 4 nodes

Parameters

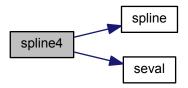
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 251 of file symbolic_functions.c.

Here is the call graph for this function:



8.6.3.11 double spline_pos4 (double t, double t, double p, double t, double t,

positive spline function with 4 nodes

Parameters

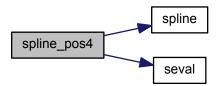
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 295 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.6.3.12 double spline5 (double t, double t1, double t1, double t2, double t2, double t3, double t3, double t4, double t4, double t5, double t5, double t6, int t8, double t9, int t8, double t9, int t8, double t9, int t8, double t9, doub

spline function with 5 nodes

Parameters

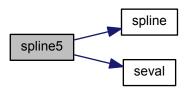
point at which the spline should be evaluated
location of node 1
spline value at node 1
location of node 2
spline value at node 2
location of node 3
spline value at node 3
location of node 4
spline value at node 4
location of node 5
spline value at node 5
flag indicating whether slope at first node should be user defined
user defined slope at first node

Returns

spline(t)

Definition at line 347 of file symbolic_functions.c.

Here is the call graph for this function:



8.6.3.13 double spline_pos5 (double t, double t, double p, double t, double t,

positive spline function with 5 nodes

Parameters

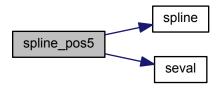
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 395 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.6.3.14 double spline10 (double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, double *t*4, double *p*4, double *t*5, double *p*5, double *t*6, double *p*6, double *t*7, double *p*7, double *t*8, double *p*8, double *t*9, double *p*9, double *t*10, double *p*10, int *ss*, double *dudt*)

spline function with 10 nodes

Parameters

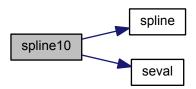
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
р3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
t6	location of node 6
p6	spline value at node 6
t7	location of node 7
p7	spline value at node 7
t8	location of node 8
p8	spline value at node 8
t9	location of node 9
p9	spline value at node 9
t10	location of node 10
p10	spline value at node 10
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 459 of file symbolic_functions.c.

Here is the call graph for this function:



8.6.3.15 double spline_pos10 (double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, double *t*4, double *p*4, double *t*5, double *p*5, double *t*6, double *p*6, double *t*7, double *p*7, double *t*8, double *p*8, double *t*9, double *p*9, double *t*10, double *p*10, int *ss*, double *dudt*)

positive spline function with 10 nodes

Parameters

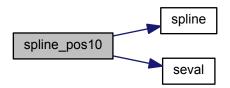
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
t6	location of node 6
p6	spline value at node 6
t7	location of node 7
р7	spline value at node 7
t8	location of node 8
p8	spline value at node 8
t9	location of node 9
р9	spline value at node 9
t10	location of node 10
p10	spline value at node 10
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 527 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.6.3.16 double Dspline3 (int *id*, double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, int *ss*, double *dudt*)

parameter derivative of spline function with 3 nodes

Parameters

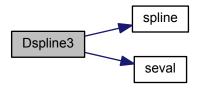
id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

dspline(t)dp(id)

Definition at line 588 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.6.3.17 double Dspline_pos3 (int *id*, double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, int *ss*, double *dudt*)

parameter derivative of positive spline function with 3 nodes

Parameters

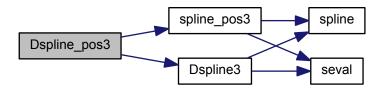
id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

dspline(t)dp(id)

Definition at line 633 of file symbolic_functions.c.

Here is the call graph for this function:



8.6.3.18 double Dspline4 (int *id*, double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, double *t*4, double *p*4, int *ss*, double *dudt*)

parameter derivative of spline function with 4 nodes

id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
SS	flag indicating whether slope at first node should be user defined

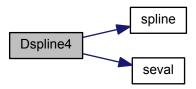
dudt	user defined slope at first node

Returns

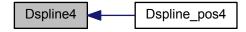
dspline(t)dp(id)

Definition at line 676 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.6.3.19 double Dspline_pos4 (int *id*, double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, double *t*4, double *p*4, int *ss*, double *dudt*)

parameter derivative of positive spline function with 4 nodes

id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4

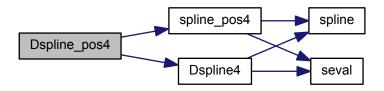
p4	spline value at node 4
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

dspline(t)dp(id)

Definition at line 725 of file symbolic_functions.c.

Here is the call graph for this function:



8.6.3.20 double Dspline5 (int id, double t, double t, double p, double t, doub

parameter derivative of spline function with 5 nodes

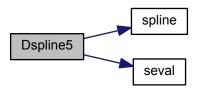
id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

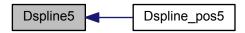
dspline(t)dp(id)

Definition at line 770 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.6.3.21 double Dspline_pos5 (int *id*, double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, double *t*4, double *p*4, double *t*5, double *p*5, int *ss*, double *dudt*)

parameter derivative of positive spline function with 5 nodes

id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
<i>p5</i>	spline value at node 5

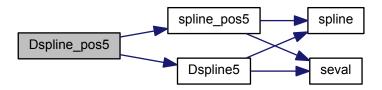
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

dspline(t)dp(id)

Definition at line 823 of file symbolic_functions.c.

Here is the call graph for this function:



8.6.3.22 double Dspline10 (int *id*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, double *t*4, double *p*4, double *t*5, double *p*5, double *t*6, double *p*6, double *t*7, double *p*7, double *t*8, double *p*8, double *t*9, double *t*10, double *p*10, int *ss*, double *dudt*)

parameter derivative of spline function with 10 nodes

id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
р1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
t6	location of node 6
p6	spline value at node 6
t7	location of node 7
р7	spline value at node 7
t8	location of node 8
p8	spline value at node 8

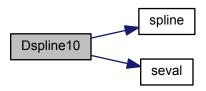
t9	location of node 9
р9	spline value at node 9
t10	location of node 10
p10	spline value at node 10
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

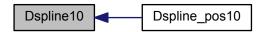
dspline(t)dp(id)

Definition at line 879 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



8.6.3.23 double Dspline_pos10 (int *id*, double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, double *t*4, double *p*4, double *t*5, double *p*5, double *t*6, double *p*6, double *t*7, double *p*7, double *t*8, double *p*8, double *t*9, double *p*9, double *t*10, double *p*10, int *ss*, double *dudt*)

parameter derivative of positive spline function with 10 nodes

id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1

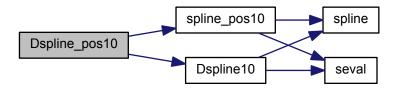
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
t6	location of node 6
p6	spline value at node 6
t7	location of node 7
p7	spline value at node 7
t8	location of node 8
p8	spline value at node 8
t9	location of node 9
р9	spline value at node 9
t10	location of node 10
p10	spline value at node 10
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

dspline(t)dp(id)

Definition at line 952 of file symbolic_functions.c.

Here is the call graph for this function:



8.7 symbolic/am_and.m File Reference

syms x y f = symfun(sym(cw_and(x,y)),[x y]); fun = f(a,b);

Functions

• mlhsInnerSubst< matlabtypesubstitute > am_and (matlabtypesubstitute a, matlabtypesubstitute b) $syms \ x \ y \ f = symfun(sym(cw_and (x, y)),[x \ y]); fun = f(a,b);$

8.8 symbolic/am_ge.m File Reference

syms x y f = symfun(sym($cw_ge(x, y)$),[x y]); fun = f(a,b);

Functions

• mlhsInnerSubst< matlabtypesubstitute > am_ge (matlabtypesubstitute a, matlabtypesubstitute b) $syms \ x \ y \ f = symfun(sym(cw_ge(x,y)),[x \ y]); \ fun = f(a,b);$

8.9 symbolic/am gt.m File Reference

```
syms x y f = symfun(sym(cw\_gt(x, y)),[x y]); fun = f(a,b);
```

Functions

• mlhsInnerSubst< matlabtypesubstitute > am_gt (matlabtypesubstitute a, matlabtypesubstitute b) $syms \ x \ y \ f = symfun(sym(cw_gt \ (x, y)),[x \ y]); fun = f(a,b);$

8.10 symbolic/am_if.m File Reference

```
syms x y z f = symfun(sym(cw_if(x, y, z)),[x y z]); fun = f(condition, truepart, falsepart);
```

Functions

mlhsInnerSubst< matlabtypesubstitute > am_if (matlabtypesubstitute condition, matlabtypesubstitute truepart, matlabtypesubstitute falsepart)

```
syms \ x \ y \ z \ f = symfun(sym(cw_if(x,y,z)),[x \ y \ z]); fun = f(condition, truepart, falsepart);
```

8.11 symbolic/am_le.m File Reference

```
syms x y f = symfun(sym(cw_le(x,y)),[x y]); fun = f(a,b);
```

Functions

mlhsInnerSubst< matlabtypesubstitute > am_le (matlabtypesubstitute a, matlabtypesubstitute b)
 syms x y f = symfun(sym(cw_le(x, y)),[x y]); fun = f(a,b);

8.12 symbolic/am_lt.m File Reference

```
syms x y f = symfun(sym(cw_lt(x,y)),[x y]); fun = f(a,b);
```

Functions

mlhsInnerSubst< matlabtypesubstitute > am_lt (matlabtypesubstitute a, matlabtypesubstitute b)
 syms x y f = symfun(sym(cw_lt(x, y)),[x y]); fun = f(a,b);

8.13 symbolic/am_max.m File Reference

```
syms x y f = symfun(sym(am_max(x,y)),[x y]); fun = f(a,b);
```

Functions

mlhsInnerSubst< matlabtypesubstitute > am_max (matlabtypesubstitute a, matlabtypesubstitute b)
 syms x y f = symfun(sym(am_max (x, y)),[x y]); fun = f(a,b);

8.14 symbolic/am_min.m File Reference

```
syms x y f = symfun(sym(am_min(x,y)),[x y]); fun = f(a,b);
```

Functions

• mlhsInnerSubst< matlabtypesubstitute > am_min (matlabtypesubstitute a, matlabtypesubstitute b) $syms \ x \ y \ f = symfun(sym(am_min(x,y)),[x \ y]); fun = f(a,b);$

8.15 symbolic/am_or.m File Reference

```
syms x y f = symfun(sym(cw_or(x, y)),[x y]); fun = f(a,b);
```

Functions

mlhsInnerSubst< matlabtypesubstitute > am_or (matlabtypesubstitute a, matlabtypesubstitute b)
 syms x y f = symfun(sym(cw_or (x, y)),[x y]); fun = f(a,b);

8.16 symbolic/am_stepfun.m File Reference

```
syms x y f = symfun(sym(am_min(x,y)),[x y]); fun = f(a,b);
```

Functions

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

```
syms x y f = symfun(sym(am_min(x, y)),[x y]); fun = f(a,b);
```

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