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	1e-8
.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*x(1) + dirac(t-param3) - const2*x(2) ];
xdot(3) = [ param4*x(2) ];
```

or

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

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

For DAEs also specify the mass matrix.

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

The specification of M may depend on parameters and constants.

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

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

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

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 root function. Events are defined to happen at the roots of the root function.

```
root(1) = state1 - state2;
```

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

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);
```

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:

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

The NaN values in Sigma_Y and Sigma_T will be replaced by the specification in Standard Deviation. Data points with NaN value will be completely ignored.

Generate a constants vector:

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

Integrate:

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

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

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:

```
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 ommited

```
% 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

```
% events fire when there is a zero crossing of the root function
root = sym(zeros(2,1));
% x3 == x2
root(1) = x3 - x2;
% x3 == x1
root(2) = x3 - x1;
```

SYSTEM STRUCT

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


end
```

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

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

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 = 1e6;
% 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) ])
```

```
Time elapsed with cvodes: 0.00195
```

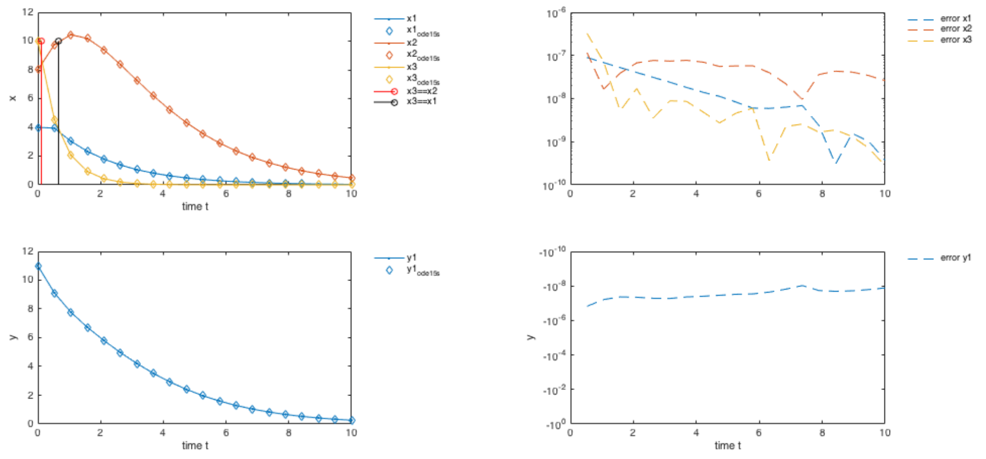
ODE15S

```
ode_system = @(t,x,p,k) [-p(1)*heaviside(t-p(4))*x(1);
    +p(2)*x(1)*exp(-0.1*t)-p(3)*x(2);
    -1.5*x(3)];
% event_fn = @(t,x) [x(3) - x(2);
%     x(3) - x(1)];
% 'Events',event_fn
options_ode15s = odeset('RelTol',1e-8,'AbsTol',1e-8,'MaxStep',1e4);

tic
[~, X_ode15s] = ode15s(@(t,x) ode_system(t,x,p,k),t,k(1:3),options_ode15s);
disp(['Time elapsed with ode15s: ' num2str(toc) ])
```

```
Time elapsed with ode15s: 0.19678
```

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_ode15s(:,ix),'d','Color',c_x(ix,:))
end
stem(sol.root(:,1),sol.root(:,1)*0+10,'r')
stem(sol.root(:,2),sol.root(:,2)*0+10,'k')
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

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);
```

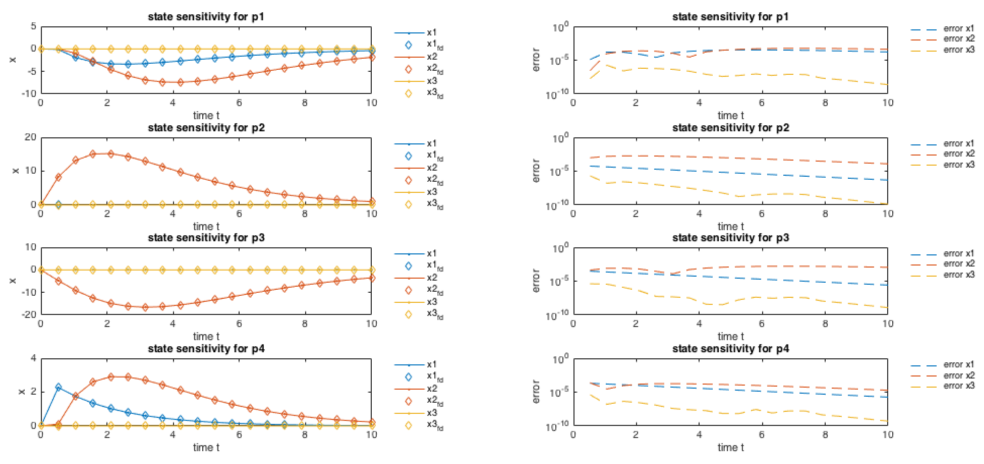
FINITE DIFFERENCES

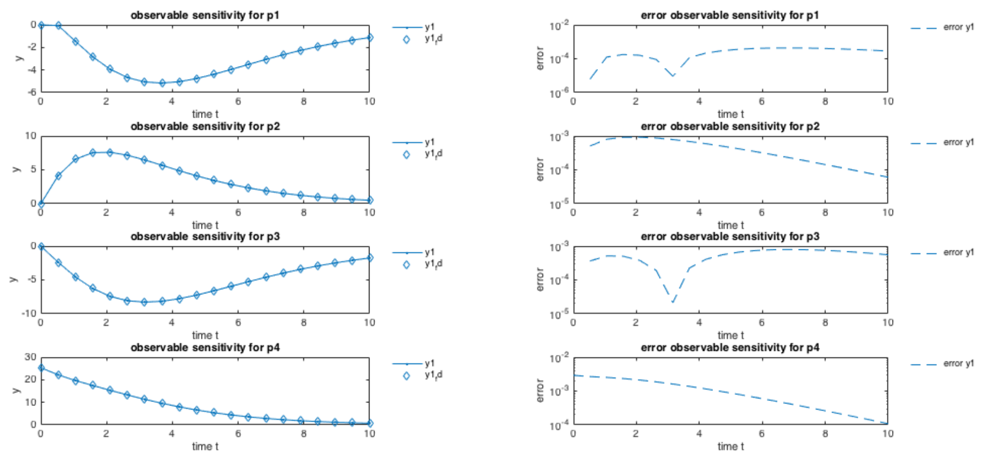
```
eps = 1e-4;
xi = log10(p);
for ip = 1:4;
    xip = xi;
    xip(ip) = xip(ip) + eps;
    solp = simulate_model_example_1(t,xip,k,[],options);
    sx_fd(:,:,ip) = (solp.x - sol.x)/eps;
    sy_fd(:,:,ip) = (solp.y - sol.y)/eps;
    sroot_fd(:,:,ip) = (solp.root - sol.root)/eps;
end
```

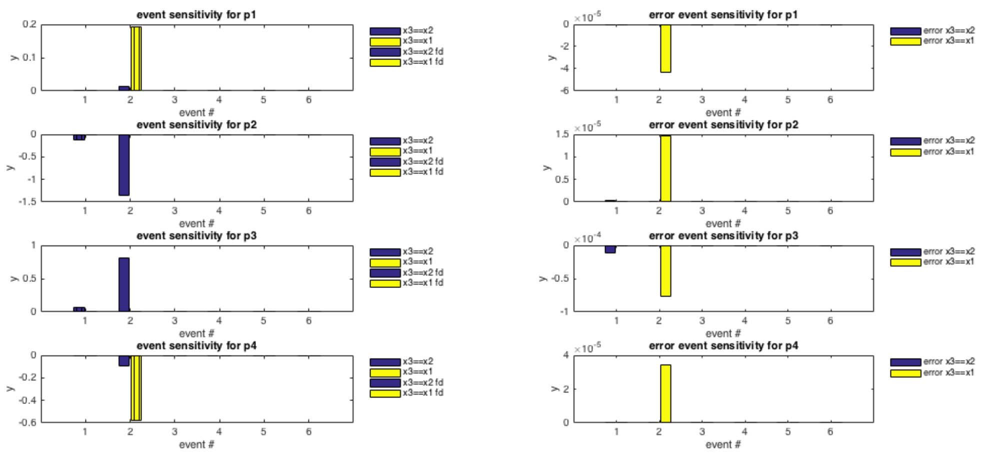
PLOTTING

```
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('x1','x1_fd','x2','x2_fd','x3','x3_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)),'--')
    legend('error x1','error x2','error x3','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,:))
    end
    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)),'--')
    legend('error y1','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(1:6,sol.sroot(1:6,:,ip),0.8)
hold on
bar(1:6,sroot_fd(1:6,:,ip),0.4)
legend('x3==x2','x3==x1','x3==x2 fd','x3==x1 fd','Location','NorthEastOutside')
legend boxoff
title(['event sensitivity for p' num2str(ip)])
xlabel('event #')
ylabel('y')
box on

subplot(4,2,2*ip)
bar(1:6,sol.sroot(1:6,:,ip)-sroot_fd(1:6,:,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('y')
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

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

```
end
```

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

3.2.2 Simulation

```
clear
```

COMPILATION

```
[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;
% load mex into memory
[msg] = which('simulate_model_example_2'); % fix for inaccessability problems
sol = simulate_model_example_2(t,log10(p),k,[],options);

tic
sol = simulate_model_example_2(t,log10(p),k,[],options);
disp(['Time elapsed with amiwrap: ' num2str(toc) ])
```

```
Time elapsed with amiwrap: 0.0019205
```

ODE15S

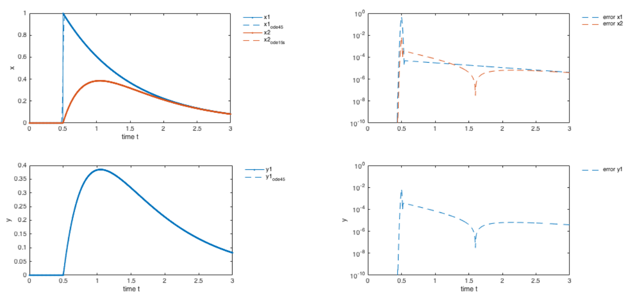
```
sig = 1e-2;
delta_num = @(tau) exp(-1/2*(tau/sig).^2)/(sqrt(2*pi)*sig);

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
[~, 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,:))
end

legend('x1','x1_ode45','x2','x2_ode15s','Location','NorthEastOutside')
legend boxoff
xlabel('time t')
ylabel('x')
box on
subplot(2,2,2)
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,:))
hold on
plot(t,X_ode45(:,2),'--','Color',c_x(1,:))
legend('y1','y1_ode45','Location','NorthEastOutside')
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

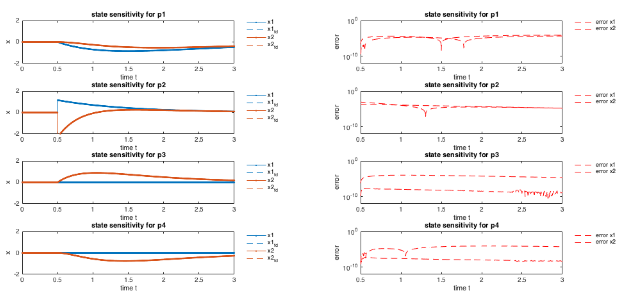
```
options.sensi = 1;

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

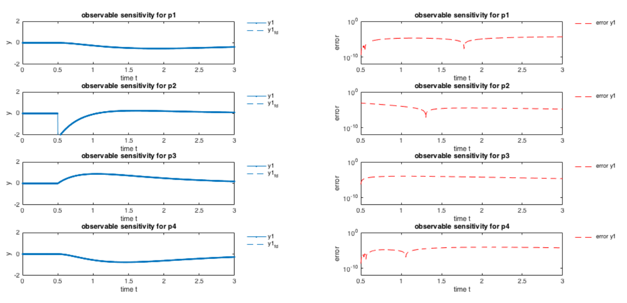
FINITE DIFFERENCES

```
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
```

PLOTTING

```
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),'--','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')
    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),'--','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
    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 ommited

```
% 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;


end
```

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

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) ])
```

```
Time elapsed with cvodes: 0.002146
```

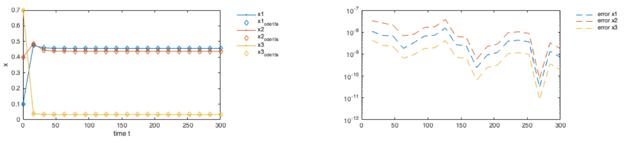
ODE15S

```
ode_system = @(t,x,p,k) [-2*p(1)*x(1)^2 - p(2)*x(1)*x(2) + 2*p(3)*x(2) + p(4)*x(3) + p(5);
    + p(1)*x(1)^2 - p(2)*x(1)*x(2) - p(3)*x(2) + p(4)*x(3);
    + p(2)*x(1)*x(2) - p(4)*x(3) - k(4)*x(3)];
options_ode15s = odeset('RelTol',1e-8,'AbsTol',1e-8,'MaxStep',1e4);

tic
[~, X_ode15s] = ode15s(@(t,x) ode_system(t,x,p,k),t,k(1:3),options_ode15s);
disp(['Time elapsed with ode15s: ' num2str(toc) ])
```

```
Time elapsed with ode15s: 0.18018
```

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_ode15s(:,ix),'d','Color',c_x(ix,:))
end
legend('x1','x1_ode15s','x2','x2_ode15s','x3','x3_ode15s','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
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);
```

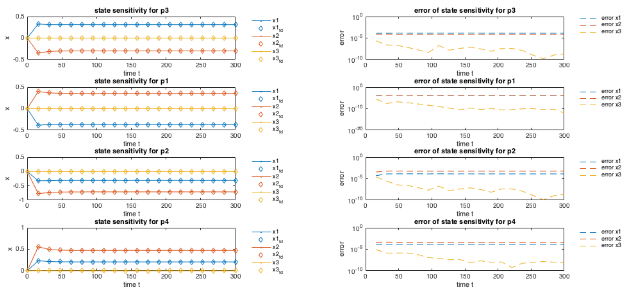
FINITE DIFFERENCES

```
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
```

PLOTTING

```
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,:))
    end
    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')
    box on

    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
end
set(gcf,'Position',[100 300 1200 500])
```



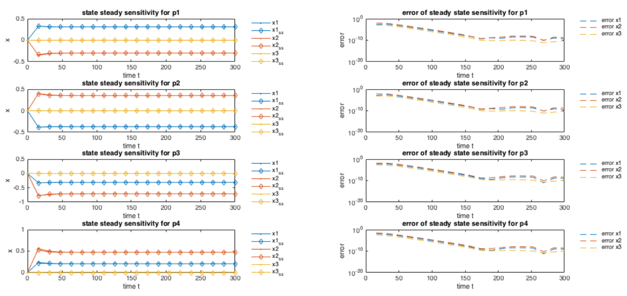
STEADY STATE SENSITIVITY

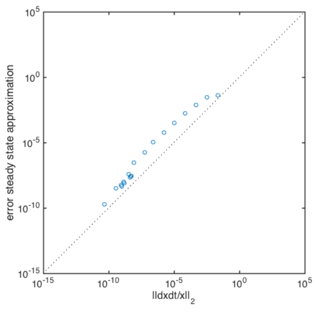
```
sssens = NaN(size(sol.sx));
for it = 2:length(t)
    tt = [0,t(it)];
    options.sensi_meth = 'ss';
    solss = simulate_model_example_3(tt,log10(p),k,[],options);
    sssens(it,:,:) = solss.sx;
    ssxdot(it,:) = solss.xdot;
end
```

PLOTTING

```
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,sssens(:,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])
```

```
figure
scatter(sqrt(sum((ssxdot./sol.x).^2,2)),sqrt(sum(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
axis square
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.atol = 1e-12;
model.rtol = 1e-8;
model.maxsteps = 1e4;
model.param = 'log10';
```

STATES

```
syms STAT pSTAT pSTAT_pSTAT npSTAT_npSTAT nSTAT1 nSTAT2 nSTAT3 nSTAT4 nSTAT5

x = [
STAT, pSTAT, pSTAT_pSTAT, npSTAT_npSTAT, nSTAT1, nSTAT2, nSTAT3, nSTAT4, nSTAT5 ...
];
```

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 sigma_pS

p = [p1,p2,p3,p4,init_STAT,sp1,sp2,sp3,sp4,sp5,offset_tSTAT,offset_pSTAT,scale_tSTAT,scale_pSTAT,sigma_pSTAT,sigma_tSTAT,sigma

k = [Omega_cyt,Omega_nuc];
```

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

```
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

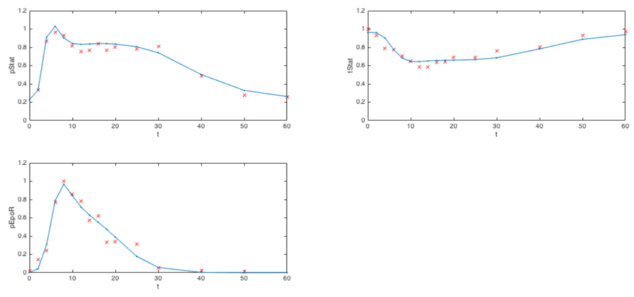
```
model.sym.x = x;
model.sym.u = u;
model.sym.xdot = xdot;
model.sym.p = p;
model.sym.k = k;
model.sym.x0 = x0;
model.sym.y = y;
model.sym.sigma_y = sigma_y;


end
```

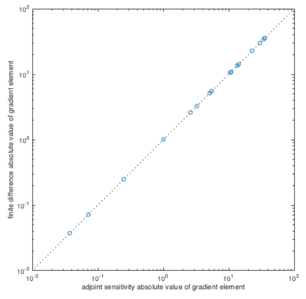
```
ans =
        atol: 1e-12
        rtol: 1e-08
    maxsteps: 10000
       param: 'log10'
         sym: [1x1 struct]
```

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
    2.99999999999997
    -0.948930681736172
    -0.00751433662124028
    0
    -2.78593598707493
    -0.256066441623149
    -0.07511250551843
    -0.411247187909784
    -4.99999999959546
    -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')
    end
    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;
end

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

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

```
% 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

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


end
```

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

3.5.2 Simulation

```
clear
```

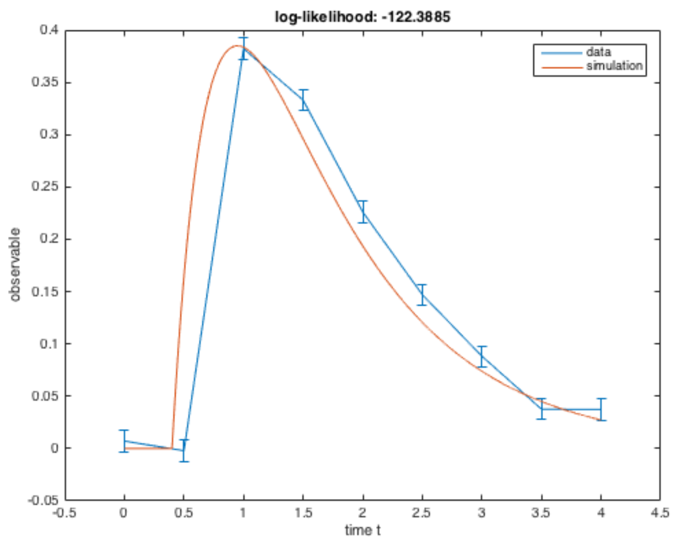
COMPILATION

```
[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

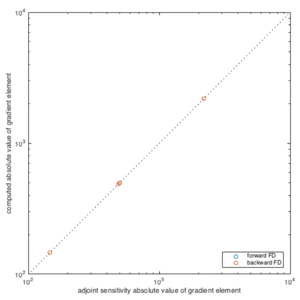
```
% time vector
tout = linspace(0,4,9);
tfine = linspace(0,4,10001);
p = [1;0.4;2;3];
k = [];

D.Y = [  0.00714742903826096
      -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([1e2,1e4])
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

```
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: 1e-08
        rtol: 1e-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)
```

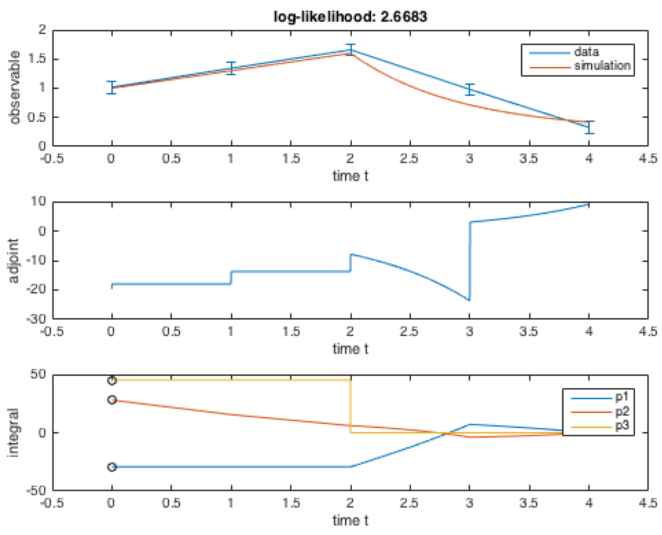
```
Generating model struct ...
Parsing model struct ...
Generating C code ...
headers | wrapfunctions |
Compiling mex file ...
Building with 'Xcode with Clang'.
MEX completed successfully.
```

SIMULATION

```
% time vector
t = [linspace(0,4,5)];
p = [1.1,0.3,1];
k = [];

% D.Y = [     1.0171
%     1.1761
%     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
%     0.5249
%     0.3288];


D.Y = [     1.0171
    1.3423
    1.6585
    0.9814
    0.3288];

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);
```

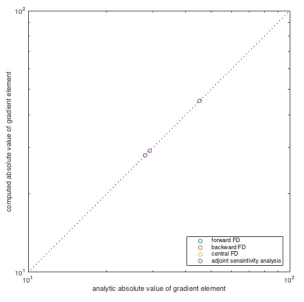
Plot

```
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) ])

y = (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);
xfine = (p(2)*tfine + 1).*(tfine<2) + ( (2*p(2)+p(3)-p(2)/p(1))*exp(-p(1)*(tfine-2))+p(2)/p(1) ).*(tfine>=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
mu = mu + ((y(it)-D.Y(it))/(D.Sigma_Y(it)^2))*exp(p(1)*(tfine-t(it))).*(tfine<=t(it)).*(tfine>2) + ((y(it)-D.Y(it))/(D.Sigma_
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)

plot(fliplr(tfine),-cumsum(fliplr(-mu.*xfine.*(tfine>2)))*p(1)*log(10)*(t(end)/numel(tfine)))
hold on
plot(fliplr(tfine),-cumsum(fliplr(mu))*p(2)*log(10)*(t(end)/numel(tfine)))
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')
```



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;
    solp = simulate_model_example_6(t,xip,k,D,options);
    grad_fd_b(ip,1) = -(solp.llh-sol.llh)/eps;
end

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([1e1,1e2],[1e1,1e2],'k:')
set(gca,'XScale','log')
set(gca,'YScale','log')
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 sym and fun fields of this object will then be populated by amimodel::parseModel(). The amimodel::sym field contains all necessary symbolic expression while the amimodel::fun field will contain flags for all functions whether the C code for a certain function needs to be regenerated or not. 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::sym (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. If changes in the dependencies occured, also the respective subfield in amimodel::fun be set to 1, indicating the necessity of regeneration of respective C code.

For all functions for which amimodel::fun is set to 1, 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 Class Index

5.1 Class List

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

6 Class Documentation

6.1 amimodel Class Reference

amimodel is the object in which all model definitions are stored

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
- mlhsInnerSubst< matlabtypesubstitute > parseModel ()

  parseModel parses the this and computes all necessary symbolic expressions.
- mlhsInnerSubst< matlabtypesubstitute > generateC ()

  generateC generates the c files which will be used in the compilation.
- mlhsInnerSubst< matlabtypesubstitute > compileC ()

  compileC compiles the mex simulation file
- mlhsInnerSubst< matlabtypesubstitute > writeCcode_sensi (::symbolic svar,::fileid fid)

  writeCcode_sensi is a wrapper for writeCcode which loops over parameters and reduces overhead by check nonzero values
- mlhsInnerSubst< matlabtypesubstitute > writeCcode (::string funstr,::fileid fid, matlabtypesubstitute ip, matlabtypesubstitute jp)

  writeCcode is a wrapper for this.gccode which initialises data and reduces overhead by check nonzero values
- mlhsInnerSubst< matlabtypesubstitute > gccode (::symbolic csym,::string funstr,::string cvar,::fileid fid)

  gccode transforms symbolic expressions into c code and writes the respective expression into a specified file
- mlhsInnerSubst< matlabtypesubstitute > generateM (::amimodel amimodelo2)

  generateM generates the matlab wrapper for the compiled C files.
- mlhsInnerSubst< matlabtypesubstitute > getFun (::struct HTable,::string funstr)

  getFun generates symbolic expressions for the requested function.
- mlhsInnerSubst< matlabtypesubstitute > getFunDeps (::string funstr)

  getDeps returns the dependencies for the requested function/expression.
- mlhsInnerSubst< matlabtypesubstitute > getFunArgs (::string funstr)

  getfunargs returns a string which contains all input arguments for the function fun.
- mlhsInnerSubst< matlabtypesubstitute > getFunCVar (::string funstr)

  getDeps returns the c variable for the requested function.
- mlhsInnerSubst< matlabtypesubstitute > getFunSVar (::string funstr)

  getDeps returns the symbolic variable for the requested function.
- mlhsSubst< mlhsInnerSubst< matlabtypesubstitute >,mlhsInnerSubst< matlabtypesubstitute > > checkDeps (::struct HTable,::cell deps)

  checkDeps checks the dependencies of functions and populates sym fields if necessary
- mlhsSubst< mlhsInnerSubst< matlabtypesubstitute >,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.

Public Attributes

- ::struct sym

  symbolic definition struct
- ::struct fun

  struct which stores information for which functions c code needs to be generated
- ::struct strsym

  short names for symbolic variables
- ::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
- ::bool debug = false

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

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

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

  default initial time
- ::string 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 nr

  number of events
- ::int ndisc

  number of discontinuities
- ::int np

  number of parameters
- ::int nk

  number of constants
- ::∗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
- ::string 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

6.1.1 Detailed Description

Definition at line 17 of file amimodel.m.

6.1.2 Constructor & Destructor Documentation

6.1.2.1 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 293 of file amimodel.m.

6.1.3 Member Function Documentation

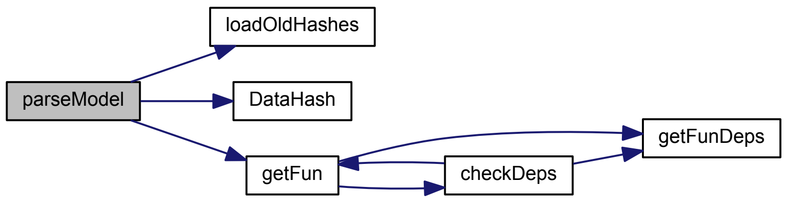
6.1.3.1 mlhsInnerSubst<::amimodel > parseModel ( )

Return values

this	updated model definition object

Definition at line 18 of file parseModel.m.

Here is the call graph for this function:



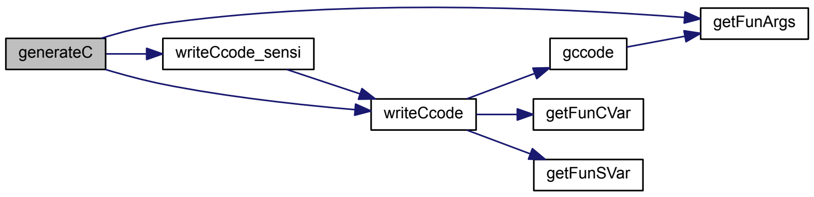
6.1.3.2 mlhsInnerSubst<::amimodel > generateC ( )

Return values

this	model definition object

Definition at line 18 of file generateC.m.

Here is the call graph for this function:



6.1.3.3 mlhsInnerSubst<::amimodel > compileC ( )

Return values

this	model definition object

Definition at line 18 of file compileC.m.

6.1.3.4 mlhsInnerSubst<::amimodel > writeCcode_sensi (::symbolic *svar,* ::fileid *fid*)

Parameters

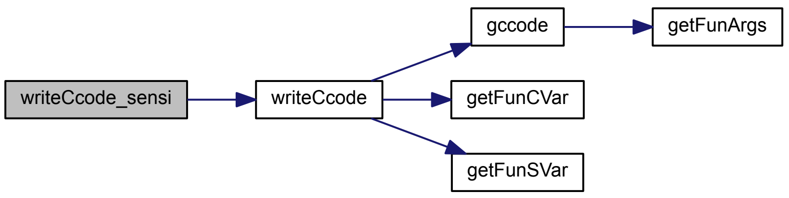
svar	symbolic variable which is later on passed to ggode
fid	file id in which the final expression is written

Return values

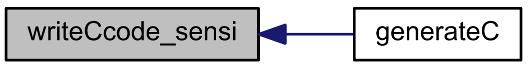
this	model definition object

Definition at line 18 of file writeCcode_sensi.m.

Here is the call graph for this function:



Here is the caller graph for this function:



6.1.3.5 mlhsInnerSubst< ::amimodel > writeCcode (::string *funstr,* ::fileid *fid,* matlabtypesubstitute *ip,* matlabtypesubstitute *jp*)

Parameters

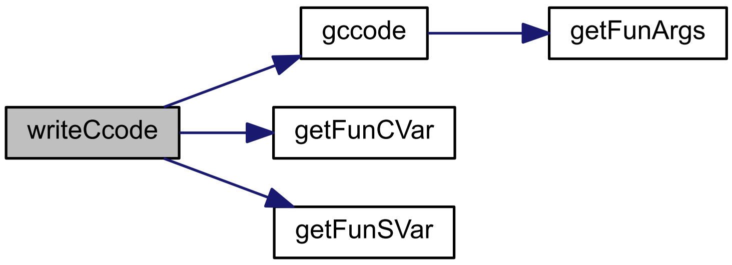
funstr	function for which C code is to be generated
fid	file id in which the final expression is written
ip	index for symbolic variable, if applicable svar(:,ip) will be passed to ggcode
jp	index for symbolic variable, if applicable svar(:,ip,jp) will be passed to ggcode

Return values

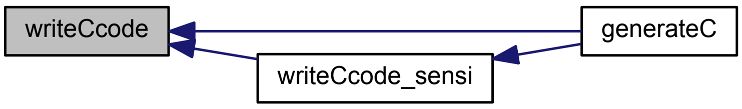
this	model definition object

Definition at line 18 of file writeCcode.m.

Here is the call graph for this function:



Here is the caller graph for this function:



6.1.3.6 mlhsInnerSubst<::amimodel > gccode (::symbolic *csym*, ::string *funstr*, ::string *cvar*, ::fileid *fid*)

Parameters

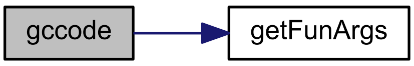
csym	symbolic expression to be transform
funstr	function for which C code is to be generated
cvar	name of the assigned variable in C
fid	file id in which the expression should be written

Return values

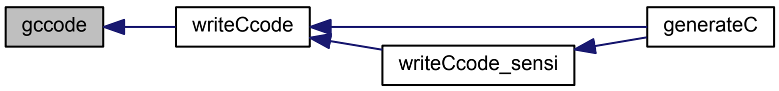
this	model definition object

Definition at line 18 of file gccode.m.

Here is the call graph for this function:



Here is the caller graph for this function:



6.1.3.7 mlhsInnerSubst<::amimodel > generateM (::amimodel *amimodelo2*)

Parameters

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

Return values

this	model definition object

Definition at line 18 of file generateM.m.

6.1.3.8 mlhsInnerSubst<::amimodel > getFun (::struct *HTable,* ::string *funstr*)

Parameters

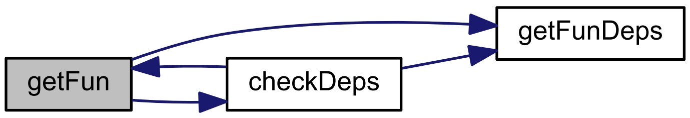
HTable	struct with hashes of symbolic definition from the previous compilation
funstr	function for which symbolic expressions should be computed

Return values

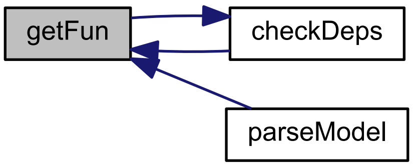
this	updated model definition object

Definition at line 18 of file getFun.m.

Here is the call graph for this function:



Here is the caller graph for this function:



6.1.3.9 mlhsInnerSubst< ::cell > getFunDeps (::string *funstr*)

Parameters

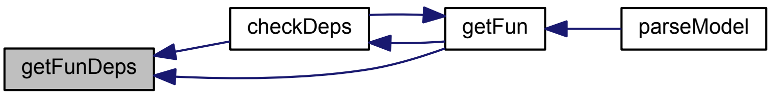
funstr	function or expression for which the dependencies should be returned

Return values

deps	cell array of dependencies

Definition at line 18 of file getFunDeps.m.

Here is the caller graph for this function:



6.1.3.10 mlhsInnerSubst< matlabtypesubstitute > getFunArgs (::string *funstr*)

Parameters

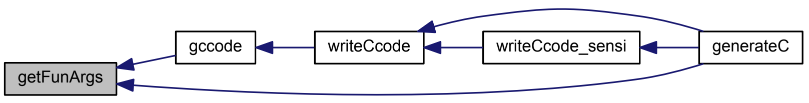
funstr	function name

Return values

str	string containing function arguments

Definition at line 18 of file getFunArgs.m.

Here is the caller graph for this function:



6.1.3.11 mlhsInnerSubst< ::string > getFunCVar (::string *funstr*)

Parameters

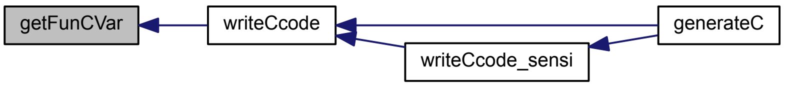
funstr	function or expression for which the dependencies should be returned

Return values

cvar	cell array of dependencies

Definition at line 18 of file getFunCVar.m.

Here is the caller graph for this function:



6.1.3.12 mlhsInnerSubst< matlabtypesubstitute > getFunSVar (::string *funstr*)

Parameters

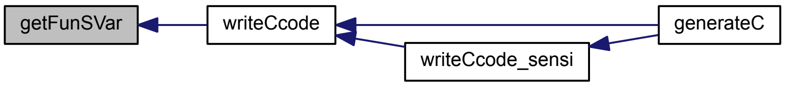
funstr	function or expression for which the dependencies should be returned

Return values

cvar	cell array of dependencies

Definition at line 18 of file getFunSVar.m.

Here is the caller graph for this function:



6.1.3.13 mlhsSubst< mlhsInnerSubst< matlabtypesubstitute >,mlhsInnerSubst< ::HTable > > 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

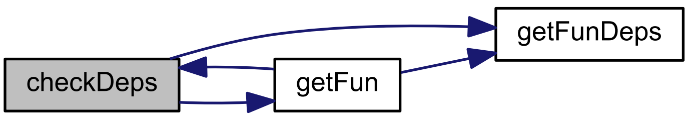
Return values

cflag	boolean indicating whether any of the dependencies have

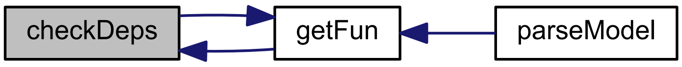
changed with respect to the hashes stored in HTable

Definition at line 18 of file checkDeps.m.

Here is the call graph for this function:



Here is the caller graph for this function:



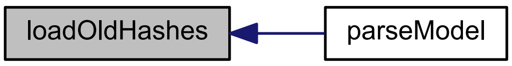
6.1.3.14 mlhsSubst< mlhsInnerSubst<::**amimodel** >,mlhsInnerSubst<::struct > > loadOldHashes ( )

Return values

this	updated model definition object
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:



6.1.3.15 mlhsInnerSubst<::amimodel > 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.

6.1.4 Member Data Documentation

6.1.4.1 atol = 1e-8

Default: 1e-8

Definition at line 61 of file amimodel.m.

6.1.4.2 rtol = 1e-8

Default: 1e-8

Definition at line 69 of file amimodel.m.

6.1.4.3 maxsteps = 1e4

Default: 1e4

Definition at line 77 of file amimodel.m.

6.1.4.4 debug = false

Default: false

Definition at line 85 of file amimodel.m.

6.1.4.5 adjoint = true

Default: true

Definition at line 93 of file amimodel.m.

6.1.4.6 forward = true

Default: true

Definition at line 101 of file amimodel.m.

6.1.4.7 t0 = 0

Default: 0

Definition at line 109 of file amimodel.m.

6.1.4.8 nxtrue = 0

Default: 0

Definition at line 131 of file amimodel.m.

6.1.4.9 nytrue = 0

Default: 0

Definition at line 146 of file amimodel.m.

6.1.4.10 coptim = "-O3"

Default: "-O3"

Definition at line 259 of file amimodel.m.

6.1.4.11 param = "lin"

Default: "lin"

Definition at line 267 of file amimodel.m.

6.1.4.12 recompile = false

Default: false

Definition at line 282 of file amimodel.m.

6.2 ExpData Struct Reference

struct that carries all information about experimental data

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

Public Attributes

- double ∗ am_my
- double ∗ am_ysigma
- double ∗ am_mt
- double ∗ am_tsigma

6.2.1 Detailed Description

Definition at line 18 of file edata.h.

6.2.2 Member Data Documentation

6.2.2.1 double∗ am_my

observed data

Definition at line 20 of file edata.h.

6.2.2.2 double∗ am_ysigma

standard deviation of observed data

Definition at line 22 of file edata.h.

6.2.2.3 double∗ am_mt

observed events

Definition at line 25 of file edata.h.

6.2.2.4 double∗ am_tsigma

standard deviation of observed events

Definition at line 27 of file edata.h.

6.3 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_rootdata
- double ∗ am_rootSdata
- double ∗ am_rootS2data
- double ∗ am_rootvaldata
- double ∗ am_rootvalSdata
- double ∗ am_rootvalS2data
- 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_llhSdata
- double ∗ am_llhS2data

6.3.1 Detailed Description

Definition at line 42 of file rdata.h.

6.3.2 Member Data Documentation

6.3.2.1 double∗ am_tsdata

timepoints

Definition at line 45 of file rdata.h.

6.3.2.2 double∗ am_xdotdata

time derivative

Definition at line 47 of file rdata.h.

6.3.2.3 double∗ am_dxdotdpdata

parameter derivative of time derivative

Definition at line 49 of file rdata.h.

6.3.2.4 double∗ am_dydxdata

state derivative of observables

Definition at line 51 of file rdata.h.

6.3.2.5 double∗ am_dydpdata

parameter derivative of observables

Definition at line 53 of file rdata.h.

6.3.2.6 double∗ am_Jdata

Jacobian of differential equation right hand side

Definition at line 55 of file rdata.h.

6.3.2.7 double∗ am_rootdata

events

Definition at line 57 of file rdata.h.

6.3.2.8 double∗ am_rootSdata

parameter derivative of events

Definition at line 59 of file rdata.h.

6.3.2.9 double∗ am_rootS2data

second order parameter derivative of events

Definition at line 61 of file rdata.h.

6.3.2.10 double∗ am_rootvaldata

value of event function

Definition at line 63 of file rdata.h.

6.3.2.11 double∗ am_rootvalSdata

parameter derivative of event function

Definition at line 65 of file rdata.h.

6.3.2.12 double∗ am_rootvalS2data

second order parameter derivative of event function

Definition at line 67 of file rdata.h.

6.3.2.13 double∗ am_xdata

returned vector state

Definition at line 69 of file rdata.h.

6.3.2.14 double∗ am_xSdata

parameter derivative of state

Definition at line 71 of file rdata.h.

6.3.2.15 double∗ am_ydata

observable

Definition at line 73 of file rdata.h.

6.3.2.16 double∗ am_ySdata

parameter derivative of observable

Definition at line 75 of file rdata.h.

6.3.2.17 double∗ am_numstepsdata

number of integration steps forward problem

Definition at line 78 of file rdata.h.

6.3.2.18 double∗ am_numstepsSdata

number of integration steps backward problem

Definition at line 80 of file rdata.h.

6.3.2.19 double∗ am_numrhsevalsdata

number of right hand side evaluations forward problem

Definition at line 82 of file rdata.h.

6.3.2.20 double∗ am_numrhsevalsSdata

number of right hand side evaluations backwad problem

Definition at line 84 of file rdata.h.

6.3.2.21 double∗ am_orderdata

employed order forward problem

Definition at line 86 of file rdata.h.

6.3.2.22 double∗ am_llhdata

likelihood value

Definition at line 89 of file rdata.h.

6.3.2.23 double∗ am_chi2data

chi2 value

Definition at line 91 of file rdata.h.

6.3.2.24 double∗ am_llhSdata

parameter derivative of likelihood

Definition at line 93 of file rdata.h.

6.3.2.25 double∗ am_llhS2data

second order parameter derivative of likelihood

Definition at line 95 of file rdata.h.

6.4 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_dx
- N_Vector am_xdot
- N_Vector am_xB
- N_Vector am_dxB
- N_Vector am_xQB
- N_Vector ∗ am_sx
- N_Vector ∗ am_sdx
- N_Vector am_id
- DlsMat am_Jtmp
- double ∗ am_llhS0
- double am_g
- double ∗ am_dgdp
- double ∗ am_dgdx
- double am_r
- double ∗ am_drdp
- double ∗ am_drdx
- double am_rval
- double ∗ am_drvaldp
- double ∗ am_drvaldx
- double ∗ am_dtdx
- double ∗ am_dtdp
- double ∗ am_dydp
- double ∗ am_dydx
- double ∗ am_yS0
- double ∗ am_sigma_y
- double ∗ am_dsigma_ydp
- double ∗ am_sigma_t
- double ∗ am_dsigma_tdp
- double ∗ am_x_tmp
- double ∗ am_sx_tmp
- double ∗ am_dx_tmp
- double ∗ am_sdx_tmp
- double ∗ am_xdot_tmp
- double ∗ am_xB_tmp

- double ∗ am_xQB_tmp
- double ∗ am_dxB_tmp
- double ∗ am_id_tmp
- int ∗ am_rootsfound
- double ∗ am_rootvaltmp
- int ∗ am_rootidx
- int am_which
- double ∗ am_discs
- double ∗ am_irdiscs

6.4.1 Detailed Description

Definition at line 64 of file tdata.h.

6.4.2 Member Data Documentation

6.4.2.1 realtype am_t

current time

Definition at line 66 of file tdata.h.

6.4.2.2 N_Vector am_x

state vector

Definition at line 69 of file tdata.h.

6.4.2.3 N_Vector am_dx

differential state vector

Definition at line 71 of file tdata.h.

6.4.2.4 N_Vector am_xdot

time derivative state vector

Definition at line 73 of file tdata.h.

6.4.2.5 N_Vector am_xB

adjoint state vector

Definition at line 75 of file tdata.h.

6.4.2.6 N_Vector am_dxB

differential adjoint state vector

Definition at line 77 of file tdata.h.

6.4.2.7 N_Vector am_xQB

quadrature state vector

Definition at line 79 of file tdata.h.

6.4.2.8 N_Vector∗ am_sx

sensitivity state vector array

Definition at line 81 of file tdata.h.

6.4.2.9 N_Vector∗ am_sdx

differential sensitivity state vector array

Definition at line 83 of file tdata.h.

6.4.2.10 N_Vector am_id

index indicating DAE equations vector

Definition at line 85 of file tdata.h.

6.4.2.11 DlsMat am_Jtmp

Jacobian

Definition at line 87 of file tdata.h.

6.4.2.12 double∗ am_llhS0

parameter derivative of likelihood array

Definition at line 90 of file tdata.h.

6.4.2.13 double am_g

data likelihood

Definition at line 92 of file tdata.h.

6.4.2.14 double∗ am_dgdp

parameter derivative of data likelihood

Definition at line 94 of file tdata.h.

6.4.2.15 double∗ am_dgdx

state derivative of data likelihood

Definition at line 96 of file tdata.h.

6.4.2.16 double am_r

event likelihood

Definition at line 98 of file tdata.h.

6.4.2.17 double∗ am_drdp

parameter derivative of event likelihood

Definition at line 100 of file tdata.h.

6.4.2.18 double∗ am_drdx

state derivative of event likelihood

Definition at line 102 of file tdata.h.

6.4.2.19 double am_rval

root function likelihood

Definition at line 104 of file tdata.h.

6.4.2.20 double∗ am_drvaldp

parameter derivative of root function likelihood

Definition at line 106 of file tdata.h.

6.4.2.21 double∗ am_drvaldx

state derivative of root function likelihood

Definition at line 108 of file tdata.h.

6.4.2.22 double∗ am_dtdx

state derivative of event

Definition at line 110 of file tdata.h.

6.4.2.23 double∗ am_dtdp

parameter derivative of event

Definition at line 112 of file tdata.h.

6.4.2.24 double∗ am_dydp

parameter derivative of observable

Definition at line 114 of file tdata.h.

6.4.2.25 double∗ am_dydx

state derivative of observable

Definition at line 116 of file tdata.h.

6.4.2.26 double∗ am_yS0

initial sensitivity of observable

Definition at line 118 of file tdata.h.

6.4.2.27 double∗ am_sigma_y

data standard deviation

Definition at line 120 of file tdata.h.

6.4.2.28 double∗ am_dsigma_ydp

parameter derivative of data standard deviation

Definition at line 122 of file tdata.h.

6.4.2.29 double∗ am_sigma_t

event standard deviation

Definition at line 124 of file tdata.h.

6.4.2.30 double∗ am_dsigma_tdp

parameter derivative of event standard deviation

Definition at line 126 of file tdata.h.

6.4.2.31 double∗ am_x_tmp

state array

Definition at line 129 of file tdata.h.

6.4.2.32 double∗ am_sx_tmp

sensitivity state array

Definition at line 131 of file tdata.h.

6.4.2.33 double∗ am_dx_tmp

differential state array

Definition at line 133 of file tdata.h.

6.4.2.34 double∗ am_sdx_tmp

differential sensitivity state array

Definition at line 135 of file tdata.h.

6.4.2.35 double∗ am_xdot_tmp

time derivative state array

Definition at line 137 of file tdata.h.

6.4.2.36 double∗ am_xB_tmp

differential adjoint state array

Definition at line 139 of file tdata.h.

6.4.2.37 double∗ am_xQB_tmp

quadrature state array

Definition at line 141 of file tdata.h.

6.4.2.38 double∗ am_dxB_tmp

differential adjoint state array

Definition at line 143 of file tdata.h.

6.4.2.39 double∗ am_id_tmp

index indicating DAE equations array

Definition at line 145 of file tdata.h.

6.4.2.40 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 151 of file tdata.h.

6.4.2.41 double∗ am_rootvaltmp

array of values of the root function

Definition at line 153 of file tdata.h.

6.4.2.42 int∗ am_rootidx

array of index which root has been found

Definition at line 155 of file tdata.h.

6.4.2.43 int am_which

integer for indexing of backwards problems

Definition at line 159 of file tdata.h.

6.4.2.44 double∗ am_discs

array containing the time-points of discontinuities

Definition at line 162 of file tdata.h.

6.4.2.45 double∗ am_irdiscs

array containing the index of discontinuities

Definition at line 164 of file tdata.h.

6.5 UserData Struct Reference

struct that stores all user provided data

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

Public Attributes

- int ∗ am_plist
- int am_np
- int am_ny
- int am_nx
- int am_nr
- int am_nt
- int am_ndisc
- int am_nnz
- int am_nmaxroot
- int am_nmaxdisc
- 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
- SlsMat am_J
- realtype ∗ am_dxdotdp

6.5.1 Detailed Description

Definition at line 64 of file udata.h.

6.5.2 Member Data Documentation

6.5.2.1 int∗ am_plist

parameter reordering

Definition at line 67 of file udata.h.

6.5.2.2 int am_np

number of parameters

Definition at line 69 of file udata.h.

6.5.2.3 int am_ny

number of observables

Definition at line 71 of file udata.h.

6.5.2.4 int am_nx

number of states

Definition at line 73 of file udata.h.

6.5.2.5 int am_nr

number of roots

Definition at line 75 of file udata.h.

6.5.2.6 int am_nt

number of timepoints

Definition at line 77 of file udata.h.

6.5.2.7 int am_ndisc

number of discontinuities

Definition at line 79 of file udata.h.

6.5.2.8 int am_nnz

number of nonzero entries in jacobian

Definition at line 81 of file udata.h.

6.5.2.9 int am_nmaxroot

maximal number of roots to collect

Definition at line 83 of file udata.h.

6.5.2.10 int am_nmaxdisc

maximal number of discontinuities to track

Definition at line 85 of file udata.h.

6.5.2.11 double∗ am_p

parameter array

Definition at line 88 of file udata.h.

6.5.2.12 double∗ am_k

constants array

Definition at line 90 of file udata.h.

6.5.2.13 double am_tstart

starting time

Definition at line 93 of file udata.h.

6.5.2.14 double∗ am_ts

timepoints

Definition at line 95 of file udata.h.

6.5.2.15 double∗ am_pbar

scaling of parameters

Definition at line 98 of file udata.h.

6.5.2.16 double∗ am_xbar

scaling of states

Definition at line 100 of file udata.h.

6.5.2.17 double∗ am_idlist

flag array for DAE equations

Definition at line 103 of file udata.h.

6.5.2.18 int am_sensi

flag indicating whether sensitivities are supposed to be computed

Definition at line 106 of file udata.h.

6.5.2.19 double am_atol

absolute tolerances for integration

Definition at line 108 of file udata.h.

6.5.2.20 double am_rtol

relative tolerances for integration

Definition at line 110 of file udata.h.

6.5.2.21 int am_maxsteps

maximum number of allowed integration steps

Definition at line 112 of file udata.h.

6.5.2.22 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 118 of file udata.h.

6.5.2.23 int am_sensi_meth

method for sensitivity computation

CW_FSA for forward sensitivity analysis, CW_ASA for adjoint sensitivity analysis

Definition at line 124 of file udata.h.

6.5.2.24 int am_linsol

linear solver specification

Definition at line 126 of file udata.h.

6.5.2.25 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 131 of file udata.h.

6.5.2.26 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 137 of file udata.h.

6.5.2.27 int am_iter

nonlinear solver

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

Definition at line 143 of file udata.h.

6.5.2.28 booleantype am_stldet

flag controlling stability limit detection

Definition at line 146 of file udata.h.

6.5.2.29 int am_ubw

upper bandwith of the jacobian

Definition at line 149 of file udata.h.

6.5.2.30 int am_lbw

lower bandwith of the jacobian

Definition at line 151 of file udata.h.

6.5.2.31 booleantype am_bsx0

flag for sensitivity initialisation

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

Definition at line 157 of file udata.h.

6.5.2.32 double∗ am_sx0data

sensitivity initialisation

Definition at line 160 of file udata.h.

6.5.2.33 int am_event_model

error model for events

Definition at line 163 of file udata.h.

6.5.2.34 int am_data_model

error model for udata

Definition at line 165 of file udata.h.

6.5.2.35 int am_ordering

state ordering

Definition at line 168 of file udata.h.

6.5.2.36 SlsMat am_J

tempory storage of Jacobian data across functions

Definition at line 171 of file udata.h.

6.5.2.37 realtype∗ am_dxdotdp

tempory storage of dxdotdp data across functions

Definition at line 173 of file udata.h.

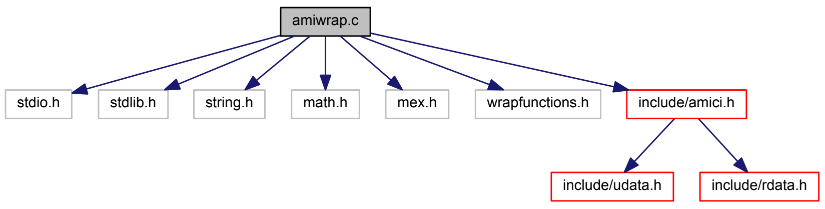
7 File Documentation

7.1 amiwrap.c File Reference

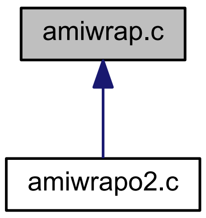
core routines for mex interface

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

Functions

- void mexFunction (int nlhs, mxArray ∗plhs[ ], int nrhs, const mxArray ∗prhs[ ])

7.1.1 Detailed Description

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

7.1.2 Function Documentation

7.1.2.1 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

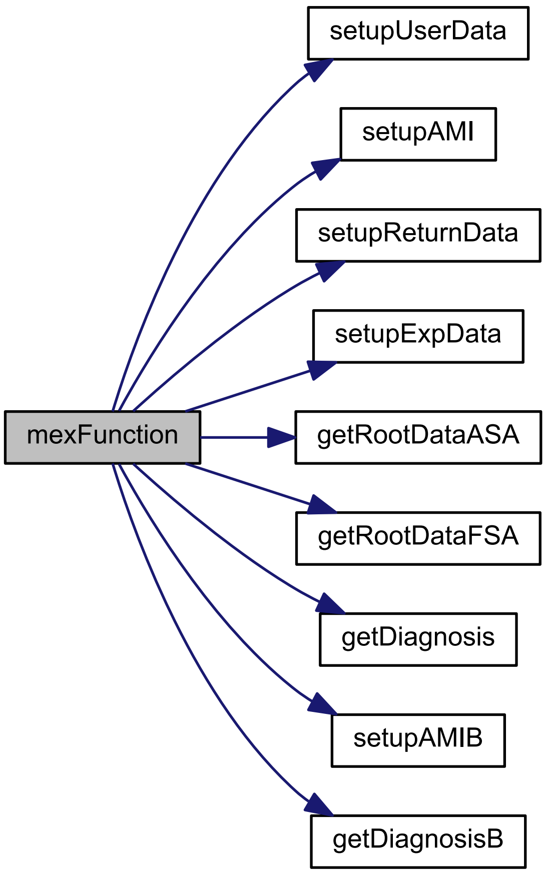
in	*nlhs*	number of output arguments of the matlab call **Type**: int
out	*plhs*	pointer to the array of output arguments **Type**: mxArray
in	*nrhs*	number of input arguments of the matlab call **Type**: int
in	*prhs*	pointer to the array of input arguments **Type**: mxArray

Returns

void

Definition at line 29 of file amiwrap.c.

Here is the call graph for this function:



7.2 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.

7.2.1 Function Documentation

7.2.1.1 noret::substitute amiwrap (matlabtypesubstitute *varargin*)

Parameters

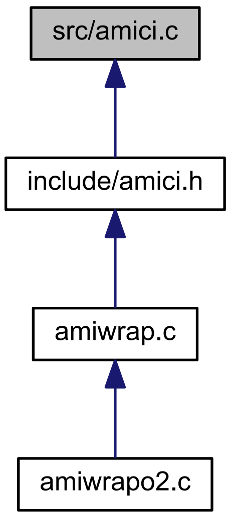
varargin	`amiwrap ( modelname, symfun, tdir, o2flag )` *Required Parameters for varargin:* • modelname specifies the name of the model which will be later used for the naming of the simualation file • symfun specifies a function which executes model defition see Model Definition for details • tdir target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

Definition at line 17 of file amiwrap.m.

7.3 src/amici.c File Reference

core routines for integration

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



Macros

- #define amici_c
- #define AMI_SUCCESS 0

Functions

- UserData setupUserData (const mxArray ∗prhs[ ])
- void ∗ setupAMI (int ∗status, void ∗user_data, void ∗temp_data)
- void setupAMIB (int ∗status, void ∗ami_mem, void ∗user_data, void ∗temp_data)
- ReturnData setupReturnData (const mxArray ∗prhs[ ], void ∗user_data)
- ExpData setupExpData (const mxArray ∗prhs[ ], void ∗user_data)
- void getRootDataFSA (int ∗status, int ∗nroots, void ∗ami_mem, void ∗user_data, void ∗return_data, void ∗temp_data)
- void getRootDataASA (int ∗status, int ∗nroots, int ∗idisc, void ∗ami_mem, void ∗user_data, void ∗return_data, void ∗exp_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)

7.3.1 Macro Definition Documentation

7.3.1.1 #define amici_c

include guard

Definition at line 8 of file amici.c.

7.3.1.2 #define AMI_SUCCESS 0

return value indicating successful execution

Definition at line 10 of file amici.c.

7.3.2 Function Documentation

7.3.2.1 UserData setupUserData (const mxArray ∗ *prhs[ ]*)

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

Parameters

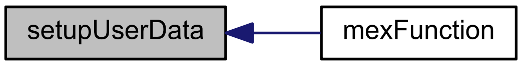
`in`	*prhs*	pointer to the array of input arguments **Type**: mxArray

Returns

udata: struct containing all provided user data

Definition at line 12 of file amici.c.

Here is the caller graph for this function:



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

setupAMIs initialises the ami memory object

Parameters

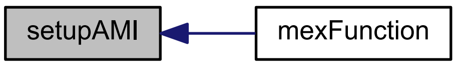
out	*status*	flag indicating success of execution **Type**: *int
in	*user_data*	pointer to the user data struct **Type**: UserData
in	*temp_data*	pointer to the temporary data struct **Type**: TempData

Returns

void

Definition at line 160 of file amici.c.

Here is the caller graph for this function:



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

setupAMIB initialises the AMI memory object for the backwards problem

Parameters

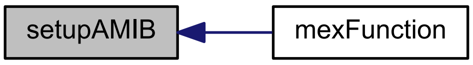
out	*status*	flag indicating success of execution **Type**: ∗int
in	*ami_mem*	pointer to the solver memory object of the forward problem
in	*user_data*	pointer to the user data struct **Type**: UserData
in	*temp_data*	pointer to the temporary data struct **Type**: TempData

Returns

void

Definition at line 444 of file amici.c.

Here is the caller graph for this function:



7.3.2.4 **ReturnData setupReturnData (const mxArray** ∗ ***prhs[ ],* void** ∗ ***user_data*)**

setupReturnData initialises the return data struct

Parameters

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

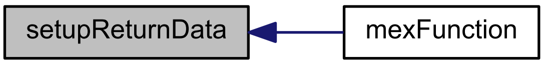
Returns

rdata: return data struct
Type: ReturnData

user udata

Definition at line 635 of file amici.c.

Here is the caller graph for this function:



7.3.2.5 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

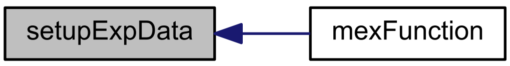
Returns

edata: experimental data struct
Type: ExpData

user udata

Definition at line 700 of file amici.c.

Here is the caller graph for this function:



7.3.2.6 void getRootDataFSA (int ∗ *status,* int ∗ *nroots,* void ∗ *ami_mem,* void ∗ *user_data,* void ∗ *return_data,* void ∗ *temp_data*)

getRootDataFSA extracts root information for forward sensitivity analysis

Parameters

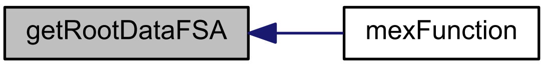
out	*status*	flag indicating success of execution **Type**: int
out	*nroots*	counter for the number of found roots **Type**: int
in	*ami_mem*	pointer to the solver memory block **Type**: void
in	*user_data*	pointer to the user data struct **Type**: UserData
out	*return_data*	pointer to the return data struct **Type**: ReturnData
out	*temp_data*	pointer to the temporary data struct **Type**: TempData

Returns

void

Definition at line 799 of file amici.c.

Here is the caller graph for this function:



7.3.2.7 void getRootDataASA (int ∗ *status*, int ∗ *nroots*, int ∗ *idisc*, void ∗ *ami_mem*, void ∗ *user_data*, void ∗ *return_data*, void ∗ *exp_data*, void ∗ *temp_data*)

getRootDataASA extracts root information for adjoint sensitivity analysis

Parameters

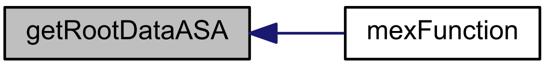
out	*status*	flag indicating success of execution **Type**: ∗int
out	*nroots*	counter for the number of found roots **Type**: ∗int
out	*idisc*	counter for the number of found discontinuities **Type**: ∗int
in	*ami_mem*	pointer to the solver memory block **Type**: ∗void
in	*user_data*	pointer to the user 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 888 of file amici.c.

Here is the caller graph for this function:



7.3.2.8 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

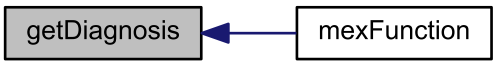
out	*status*	flag indicating success of execution **Type**: ∗int
in	*it*	time-point index **Type**: int
in	*ami_mem*	pointer to the solver memory block **Type**: ∗void
in	*user_data*	pointer to the user data struct **Type**: UserData
out	*return_data*	pointer to the return data struct **Type**: ReturnData

Returns

void

Definition at line 1003 of file amici.c.

Here is the caller graph for this function:



7.3.2.9 void getDiagnosisB (int ∗ *status*, int *it*, void ∗ *ami_mem*, void ∗ *user_data*, void ∗ *return_data*, void ∗ *temp_data*)

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

Parameters

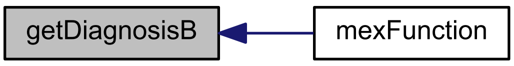
out	*status*	flag indicating success of execution **Type**: ∗int
in	*it*	time-point index **Type**: int
in	*ami_mem*	pointer to the solver memory block **Type**: ∗void
in	*user_data*	pointer to the user data struct **Type**: UserData
out	*return_data*	pointer to the return data struct **Type**: ReturnData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

Returns

void

Definition at line 1037 of file amici.c.

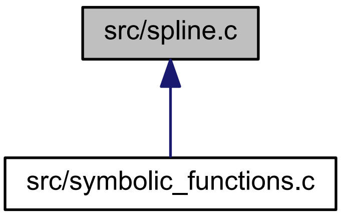
Here is the caller graph for this function:



7.4 src/spline.c File Reference

definition of spline functions

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



Functions

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

7.4.1 Detailed Description

Author

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

7.4.2 Function Documentation

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

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

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

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

Parameters

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

Return values

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

Notes

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

Definition at line 66 of file spline.c.

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

Evaluate the cubic spline function

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

Parameters

`in`	*n*	The number of data points or knots (n >= 2)
`in`	*u*	the abscissa at which the spline is to be evaluated
`in`	*x[ ]*	the abscissas of the knots in strictly increasing order

in	*y[ ]*	the ordinates of the knots
in	*b*	array of spline coefficients computed by spline().
in	*c*	array of spline coefficients computed by spline().
in	*d*	array of spline coefficients computed by spline().

Returns

the value of the spline function at u

Notes

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

Definition at line 208 of file spline.c.

7.4.2.3 double deriv (int *n*, double *u*, double *x[ ]*, double *b[ ]*, double *c[ ]*, double *d[ ]*)

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 U < X[0] then i = 0 is used. If U > X[n-1] then i = n-1 is used.

Parameters

in	*n*	the number of data points or knots (n >= 2)
in	*u*	the abscissa at which the 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	*c*	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.

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

Integrate the cubic spline function

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

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

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

Parameters

in	*n*	the number of data points or knots (n >= 2)
in	*u*	the abscissa at which the spline is to be evaluated

in	*x[ ]*	the abscissas of the knots in strictly increasing order
in	*y[ ]*	the ordinates of the knots
in	*b*	array of spline coefficients computed by spline().
in	*c*	array of spline coefficients computed by spline().
in	*d*	array of spline coefficients computed by spline().

Returns

the value of the spline function at u

Notes

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

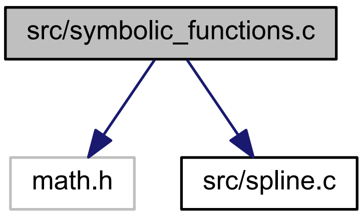
Definition at line 324 of file spline.c.

7.5 src/symbolic_functions.c File Reference

definition of symbolic functions

```
#include <math.h>
#include <src/spline.c>
```

Include dependency graph for symbolic_functions.c:



Macros

- #define amici_symbolic_functions_c
- #define TRUE 1
- #define FALSE 0

Functions

- int am_ge (double a, double b)
- int Dam_ge (int id, double a, double b)
- int am_gt (double a, double b)
- int Dam_gt (int id, double a, double b)
- int am_le (double a, double b)
- int Dam_le (int id, double a, double b)
- int am_lt (double a, double b)

- int Dam_lt (int id, double a, double b)
- double am_if (int condition, double truepart, double falsepart)
- double Dam_if (int id, int condition, double truepart, double falsepart)
- int am_and (int a, int b)
- double Dam_and (int id, int a, int b)
- int am_or (int a, int b)
- double Dam_or (int id, int a, int b)
- 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 heaviside (double x)
- double dirac (double x)
- double Ddirac (int id, double x)
- 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 p9, double t10, double p10, int ss, double dudt)

7.5.1 Detailed Description

This file contains definitions of various symbolic functions which

7.5.2 Macro Definition Documentation

7.5.2.1 #define amici_symbolic_functions_c

include guard

Definition at line 10 of file symbolic_functions.c.

7.5.2.2 #define TRUE 1

bool return value true

Definition at line 16 of file symbolic_functions.c.

7.5.2.3 #define FALSE 0

bool return value false

Definition at line 18 of file symbolic_functions.c.

7.5.3 Function Documentation

7.5.3.1 int am_ge (double *a*, double *b*)

c implementation of matlab function ge

Parameters

a	value1 **Type**: double
b	value2 **Type**: double

Returns

if(a >= 0) then 1 else 0
Type: int

Definition at line 28 of file symbolic_functions.c.

7.5.3.2 int Dam_ge (int *id*, double *a*, double *b*)

parameter derivative of c implementation of matlab function ge

Parameters

id	argument index for differentiation
a	value1 **Type**: double
b	value2 **Type**: double

Returns

0

Definition at line 45 of file symbolic_functions.c.

7.5.3.3 int am_gt (double *a*, double *b*)

c implementation of matlab function gt

Parameters

a	value1 **Type**: double
b	value2 **Type**: double

Returns

if(a > 0) then 1 else 0
Type: int

Definition at line 57 of file symbolic_functions.c.

7.5.3.4 int Dam_gt (int *id*, double *a*, double *b*)

parameter derivative of c implementation of matlab function gt

Parameters

id	argument index for differentiation
a	value1 **Type**: double
b	value2 **Type**: double

Returns

0

Definition at line 74 of file symbolic_functions.c.

7.5.3.5 int am_le (double *a*, double *b*)

c implementation of matlab function le

Parameters

a	value1 **Type**: double
b	value2 **Type**: double

Returns

if(a <= 0) then 1 else 0
Type: int

Definition at line 86 of file symbolic_functions.c.

7.5.3.6 int Dam_le (int *id*, double *a*, double *b*)

parameter derivative of c implementation of matlab function le

Parameters

id	argument index for differentiation

a	value1 **Type**: double
b	value2 **Type**: double

Returns

0

Definition at line 103 of file symbolic_functions.c.

7.5.3.7 int am_lt (double *a*, double *b*)

c implementation of matlab function lt

Parameters

a	value1 **Type**: double
b	value2 **Type**: double

Returns

if(a $<$ 0) then 1 else 0
Type: int

Definition at line 115 of file symbolic_functions.c.

7.5.3.8 int Dam_lt (int *id*, double *a*, double *b*)

parameter derivative of c implementation of matlab function lt

Parameters

id	argument index for differentiation
a	value1 **Type**: double
b	value2 **Type**: double

Returns

0

Definition at line 132 of file symbolic_functions.c.

7.5.3.9 double am_if (int *condition*, double *truepart*, double *falsepart*)

c implementation of if function

Parameters

condition	condition that decides on the output
truepart	returnvalue if condition is true **Type**: double

falsepart	returnvalue if condition is false **Type**: double

Returns

if(condition) then truepart else falsepart
Type: int

Definition at line 145 of file symbolic_functions.c.

7.5.3.10 double Dam_if (int *id,* int *condition,* double *truepart,* double *falsepart*)

parameter derivative of c implementation of if function

Parameters

id	argument index for differentiation
condition	condition that decides on the output
truepart	returnvalue if condition is true **Type**: double
falsepart	returnvalue if condition is false **Type**: double

Returns

id==1: 0
Type: double
id==2: if(condition) then 1 else 0
Type: double
id==3: if(condition) then 0 else 1
Type: double

Definition at line 166 of file symbolic_functions.c.

7.5.3.11 int am_and (int *a,* int *b*)

c implementation of matlab function and

Parameters

a	bool1 **Type**: int
b	bool2 **Type**: int

Returns

if(a & b) then 1 else 0
Type: int

Definition at line 200 of file symbolic_functions.c.

7.5.3.12 double Dam_and (int *id,* int *a,* int *b*)

parameter derivative of c implementation of matlab function and

Parameters

id	argument index for differentiation
a	bool1 **Type**: int
b	bool2 **Type**: int

Returns

0
Type: double

Definition at line 217 of file symbolic_functions.c.

7.5.3.13 int am_or (int *a*, int *b*)

c implementation of matlab function or

Parameters

a	bool1 **Type**: int
b	bool2 **Type**: int

Returns

if(a | b) then 1 else 0
Type: int

Definition at line 229 of file symbolic_functions.c.

7.5.3.14 double Dam_or (int *id*, int *a*, int *b*)

parameter derivative of c implementation of matlab function or

Parameters

id	argument index for differentiation
a	bool1 **Type**: int
b	bool2 **Type**: int

Returns

0
Type: double

Definition at line 246 of file symbolic_functions.c.

7.5.3.15 double am_min (double *a*, double *b*)

c implementation of matlab function min

Parameters

a	value1 **Type**: double
b	value2 **Type**: double

Returns

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

Definition at line 258 of file symbolic_functions.c.

7.5.3.16 double Dam_min (int *id*, double *a*, double *b*)

parameter derivative of c implementation of matlab function min

Parameters

id	argument index for differentiation
a	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 276 of file symbolic_functions.c.

7.5.3.17 double am_max (double *a*, double *b*)

c implementation of matlab function min

Parameters

a	value1 **Type**: double
b	value2 **Type**: double

Returns

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

Definition at line 300 of file symbolic_functions.c.

7.5.3.18 double Dam_max (int *id*, double *a*, double *b*)

parameter derivative of c implementation of matlab function min

Parameters

id	argument index for differentiation
a	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 318 of file symbolic_functions.c.

7.5.3.19 double heaviside (double *x*)

c implementation of matlab function heaviside

Parameters

x	argument

Returns

if(x$>$0) then 1 else 0

Definition at line 341 of file symbolic_functions.c.

7.5.3.20 double dirac (double *x*)

c implementation of matlab function dirac

Parameters

x	argument

Returns

if(x==0) then 1 else 0

Definition at line 356 of file symbolic_functions.c.

7.5.3.21 double Ddirac (int *id,* double *x*)

derivatives of the c implementation of matlab function dirac

Parameters

id	argument index for differentiation
x	argument

Returns

0
Type: double

Definition at line 372 of file symbolic_functions.c.

7.5.3.22 double spline3 (double *t,* double *t1,* double *p1,* double *t2,* double *p2,* double *t3,* double *p3,* int *ss,* double *dudt*)

spline function with 3 nodes

Parameters

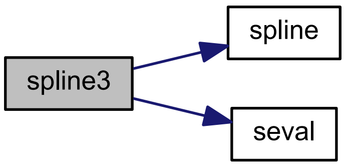
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 396 of file symbolic_functions.c.

Here is the call graph for this function:



7.5.3.23 double spline_pos3 (double *t*, double *t1*, double *p1*, double *t2*, double *p2*, double *t3*, double *p3*, int *ss*, double *dudt*)

positive spline function with 3 nodes

Parameters

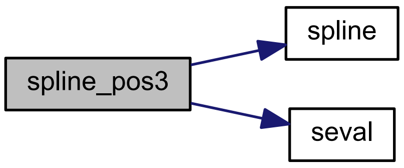
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

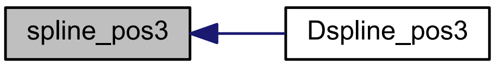
spline(t)

Definition at line 437 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



7.5.3.24 double spline4 (double *t*, double *t1*, double *p1*, double *t2*, double *p2*, double *t3*, double *p3*, double *t4*, double *p4*, int *ss*, double *dudt*)

spline function with 4 nodes

Parameters

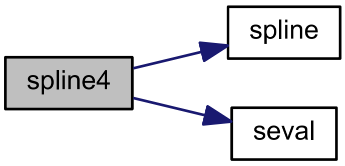
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 485 of file symbolic_functions.c.

Here is the call graph for this function:



7.5.3.25 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*)

positive spline function with 4 nodes

Parameters

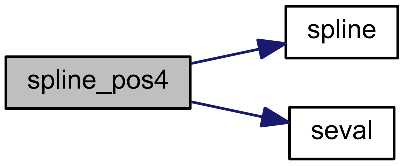
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

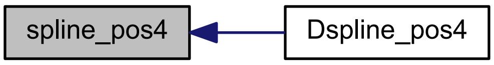
spline(t)

Definition at line 529 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



7.5.3.26 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*)

spline function with 5 nodes

Parameters

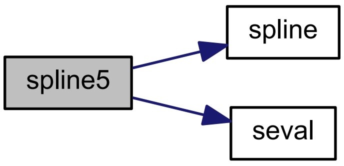
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 581 of file symbolic_functions.c.

Here is the call graph for this function:



7.5.3.27 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*)

positive spline function with 5 nodes

Parameters

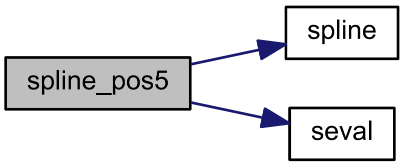
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

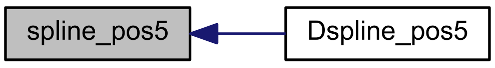
spline(t)

Definition at line 629 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



7.5.3.28 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*)

spline function with 10 nodes

Parameters

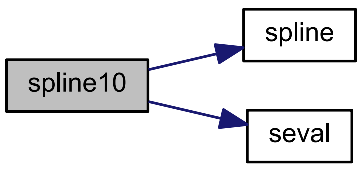
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
t6	location of 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 693 of file symbolic_functions.c.

Here is the call graph for this function:



7.5.3.29 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*)

positive spline function with 10 nodes

Parameters

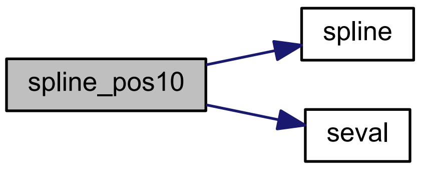
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
t6	location of 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

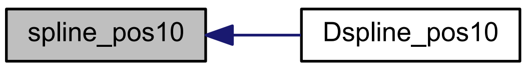
spline(t)

Definition at line 761 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



7.5.3.30 double Dspline3 (int *id,* double *t,* double *t1,* double *p1,* double *t2,* double *p2,* double *t3,* double *p3,* int *ss,* double *dudt*)

parameter derivative of spline function with 3 nodes

Parameters

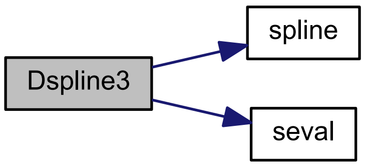
id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

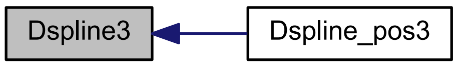
dspline(t)dp(id)

Definition at line 822 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



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

parameter derivative of positive spline function with 3 nodes

Parameters

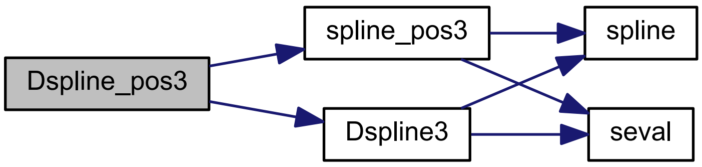
id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

dspline(t)dp(id)

Definition at line 867 of file symbolic_functions.c.

Here is the call graph for this function:



7.5.3.32 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*)

parameter derivative of spline function with 4 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
p3	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

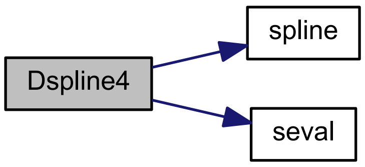
dudt	user defined slope at first node

Returns

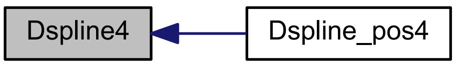
dspline(t)dp(id)

Definition at line 910 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



7.5.3.33 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*)

parameter derivative of positive spline function with 4 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
p3	spline value at node 3
t4	location of node 4

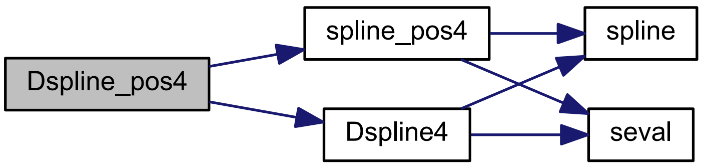
p4	spline value at node 4
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

dspline(t)dp(id)

Definition at line 959 of file symbolic_functions.c.

Here is the call graph for this function:



7.5.3.34 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*)

parameter derivative of spline function with 5 nodes

Parameters

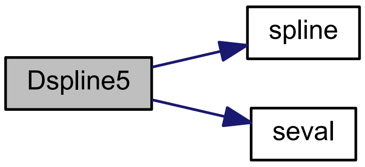
id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	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

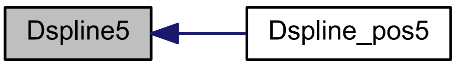
dspline(t)dp(id)

Definition at line 1004 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



7.5.3.35 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*)

parameter derivative of positive spline function with 5 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
p3	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

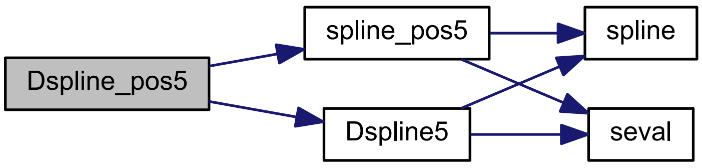
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

dspline(t)dp(id)

Definition at line 1057 of file symbolic_functions.c.

Here is the call graph for this function:



7.5.3.36 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*)

parameter derivative of spline function with 10 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
p3	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

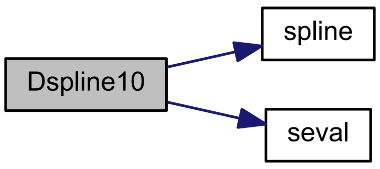
t9	location of node 9
p9	spline value at node 9
t10	location of node 10
p10	spline value at node 10
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

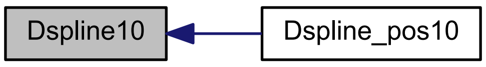
dspline(t)dp(id)

Definition at line 1113 of file symbolic_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



7.5.3.37 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 *p9*, double *t10*, double *p10*, int *ss*, double *dudt*)

parameter derivative of positive spline function with 10 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

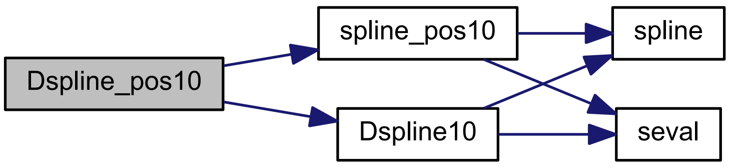
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
p3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
t6	location of node 6
p6	spline value at node 6
t7	location of node 7
p7	spline value at node 7
t8	location of 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

dspline(t)dp(id)

Definition at line 1186 of file symbolic_functions.c.

Here is the call graph for this function:



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